



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2026 – 10:36 AM EDT

PDB ID : 3JQP / pdb_00003jqp
Title : Crystal structure of the H286L mutant of Ferredoxin-NADP⁺ reductase from Plasmodium falciparum with 2'P-AMP
Authors : Canevari, G.; Milani, M.; Bolognesi, M.
Deposited on : 2009-09-07
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

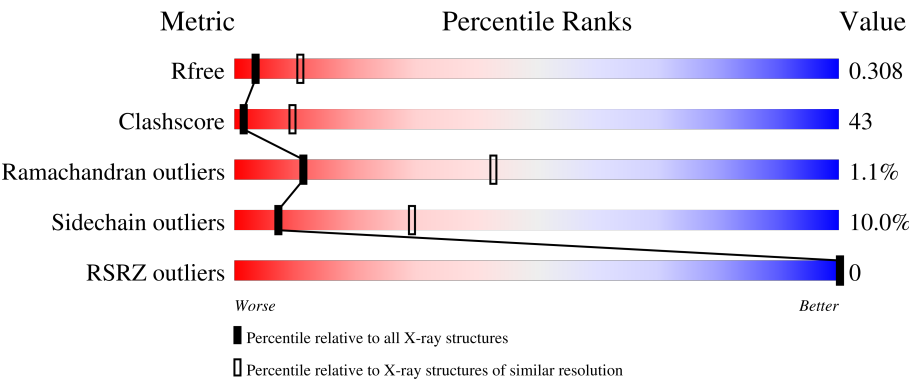
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	316	42%36%5%•16%
1	B	316	30%42%11%•16%
1	C	316	47%31%5%16%
1	D	316	43%35%6%•15%
1	E	316	40%36%6%17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	316	43%30%6%19%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13874 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.

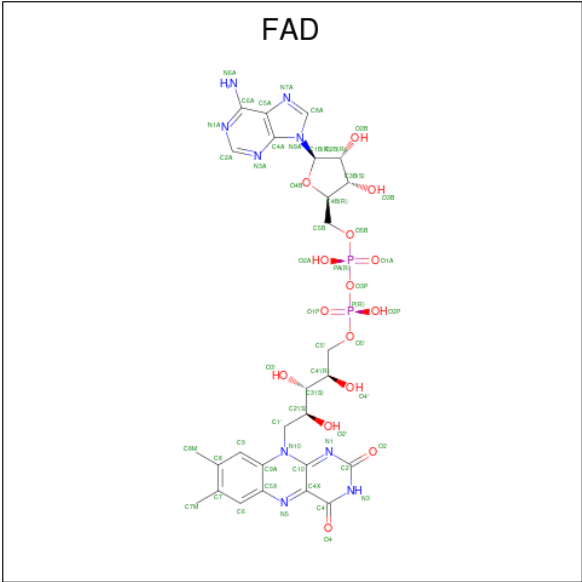
- Molecule 1 is a protein called Ferredoxin NADP reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	5	0	0
			2210	1434	363	404	9			
1	B	266	Total	C	N	O	S	0	0	0
			2231	1451	366	405	9			
1	C	265	Total	C	N	O	S	0	0	0
			2209	1433	361	406	9			
1	D	269	Total	C	N	O	S	0	0	0
			2248	1456	372	411	9			
1	E	261	Total	C	N	O	S	0	0	0
			2190	1425	357	399	9			
1	F	257	Total	C	N	O	S	0	0	0
			2140	1395	349	387	9			

There are 6 discrepancies between the modelled and reference sequences:

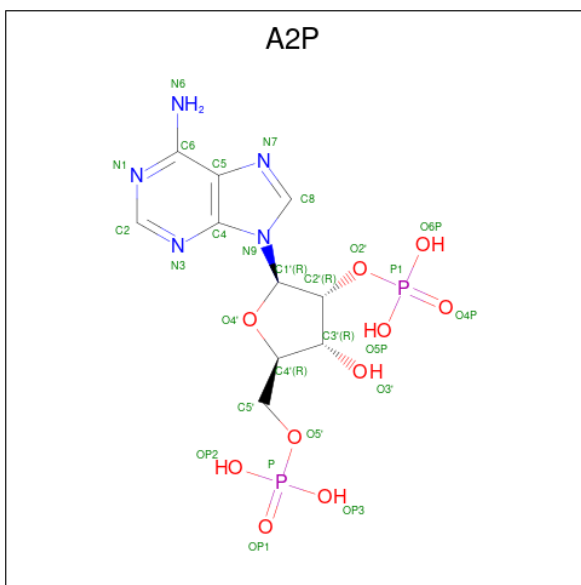
Chain	Residue	Modelled	Actual	Comment	Reference
A	286	LEU	HIS	engineered mutation	UNP C6KT68
B	286	LEU	HIS	engineered mutation	UNP C6KT68
C	286	LEU	HIS	engineered mutation	UNP C6KT68
D	286	LEU	HIS	engineered mutation	UNP C6KT68
E	286	LEU	HIS	engineered mutation	UNP C6KT68
F	286	LEU	HIS	engineered mutation	UNP C6KT68

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is ADENOSINE-2'-5'-DIPHOSPHATE (CCD ID: A2P) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

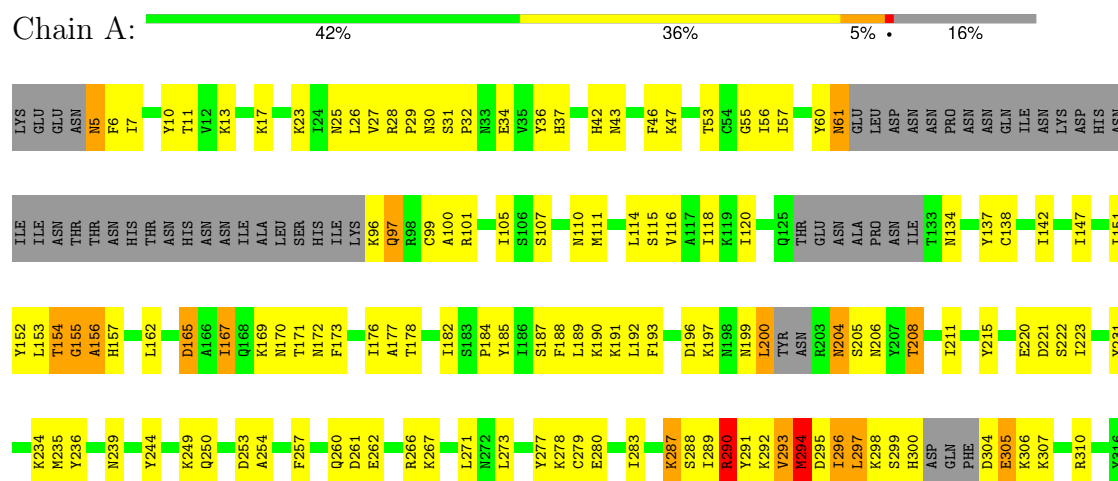
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	29	Total	O	0	0
			29	29		
4	C	29	Total	O	0	0
			29	29		
4	D	30	Total	O	0	0
			30	30		
4	E	22	Total	O	0	0
			22	22		
4	F	27	Total	O	0	0
			27	27		

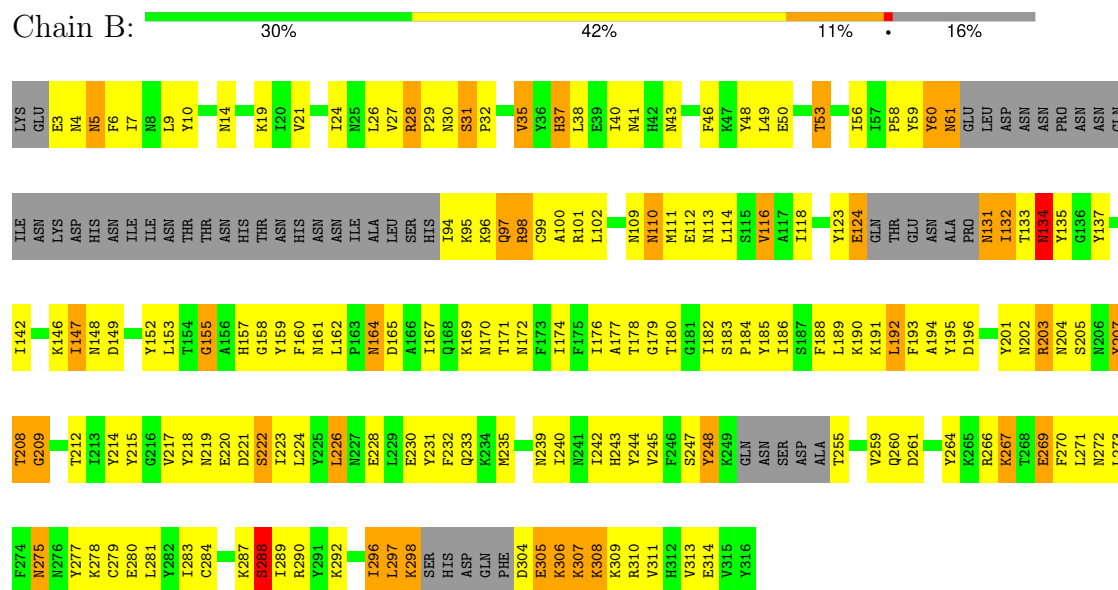
3 Residue-property plots

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: Ferredoxin NADP reductase

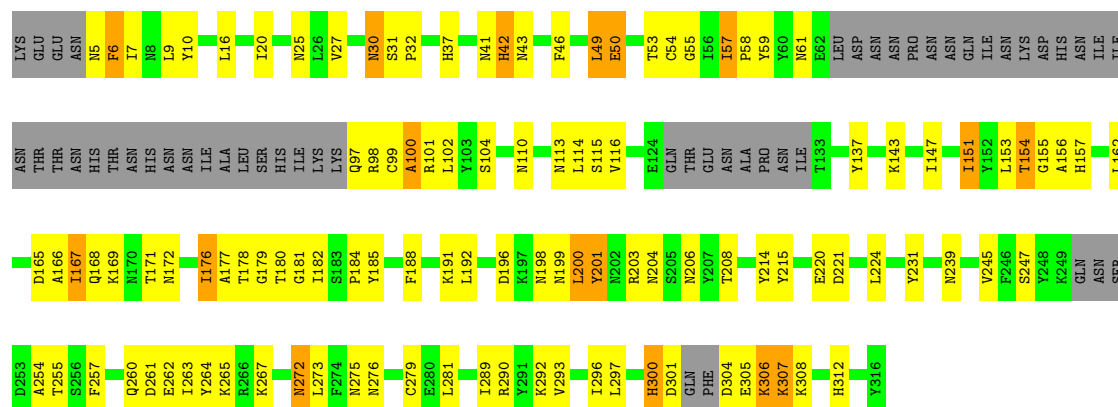


• Molecule 1: Ferredoxin NADP reductase



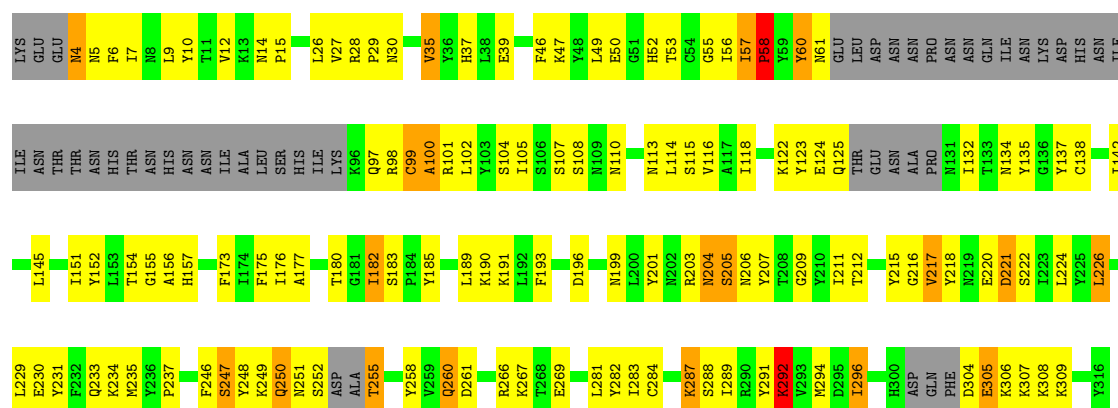
• Molecule 1: Ferredoxin NADP reductase





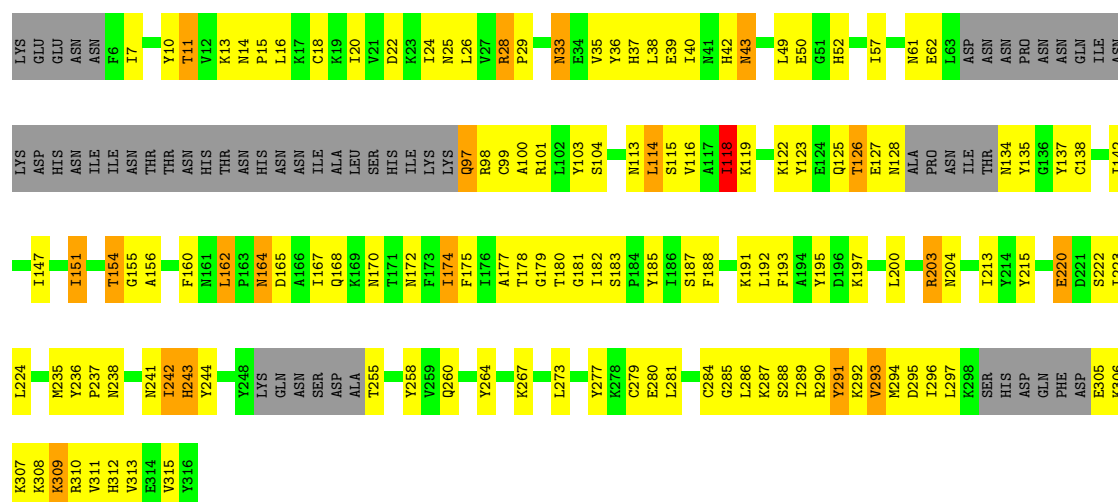
• Molecule 1: Ferredoxin NADP reductase

Chain D: 43% 35% 6% 15%



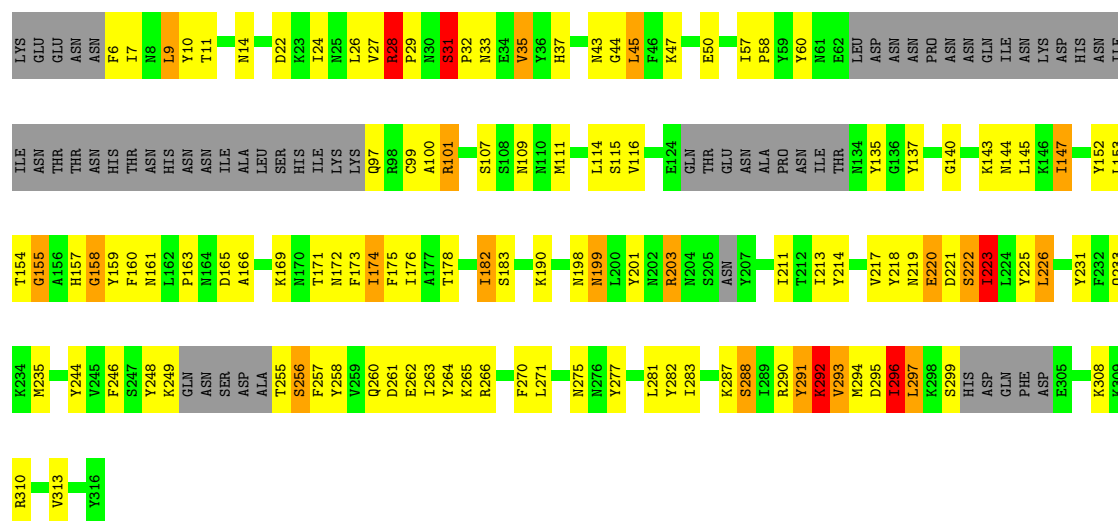
• Molecule 1: Ferredoxin NADP reductase

Chain E: 40% 36% 6% 17%



• Molecule 1: Ferredoxin NADP reductase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	122.57Å 122.57Å 133.74Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.58 – 3.00 56.58 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.58-3.00) 99.9 (56.58-3.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.244 , 0.317 0.244 , 0.308	Depositor DCC
R_{free} test set	2268 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.012 for -h,-k,l 0.449 for h,-h-k,-l 0.018 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13874	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.1827e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, A2P

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	0.52	1/2262 (0.0%)	0.89	13/3051 (0.4%)
1	B	0.63	0/2283	0.94	12/3078 (0.4%)
1	C	0.52	0/2262	0.88	5/3053 (0.2%)
1	D	0.51	0/2301	0.90	10/3104 (0.3%)
1	E	0.46	0/2242	0.93	11/3025 (0.4%)
1	F	0.62	0/2191	0.99	17/2954 (0.6%)
All	All	0.55	1/13541 (0.0%)	0.92	68/18265 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	254	ALA	C-N	-7.98	1.22	1.33

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	307	LYS	N-CA-C	-14.27	96.46	112.72
1	F	292	LYS	N-CA-C	-10.11	96.60	110.35
1	B	307	LYS	N-CA-C	-8.56	101.83	113.30
1	F	201	TYR	N-CA-C	8.42	120.46	111.28
1	A	307	LYS	N-CA-C	-8.28	102.90	113.16
1	C	198	ASN	N-CA-C	8.26	120.06	111.14
1	F	44	GLY	N-CA-C	-8.25	103.94	115.32
1	B	306	LYS	N-CA-C	-7.80	103.34	112.86
1	A	154	THR	CA-C-N	7.74	129.82	120.14
1	A	154	THR	C-N-CA	7.74	129.82	120.14
1	A	290	ARG	N-CA-C	7.69	119.74	111.36
1	D	309	LYS	N-CA-C	-7.56	103.67	113.12
1	F	31	SER	CA-C-N	7.21	128.86	119.84
1	F	31	SER	C-N-CA	7.21	128.86	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	205	SER	N-CA-C	7.07	120.09	110.55
1	F	161	ASN	N-CA-C	7.04	119.61	110.53
1	F	198	ASN	N-CA-C	6.82	118.50	111.14
1	B	134	ASN	N-CA-C	6.52	119.69	110.50
1	D	60	TYR	N-CA-C	6.52	118.98	109.07
1	F	220	GLU	N-CA-C	-6.44	104.34	111.36
1	B	308	LYS	N-CA-C	-6.26	105.39	113.16
1	B	59	TYR	N-CA-C	6.18	119.62	111.28
1	D	57	ILE	O-C-N	6.12	126.23	121.46
1	A	294	MET	N-CA-C	-6.10	103.79	111.11
1	B	60	TYR	N-CA-C	6.09	119.75	112.93
1	B	31	SER	CA-C-N	6.06	125.78	119.05
1	B	31	SER	C-N-CA	6.06	125.78	119.05
1	D	305	GLU	N-CA-C	6.03	117.65	111.14
1	A	293	VAL	N-CA-C	-5.97	106.00	111.67
1	D	206	ASN	N-CA-C	5.97	118.45	108.96
1	E	28	ARG	CA-C-N	5.85	127.15	119.84
1	E	28	ARG	C-N-CA	5.85	127.15	119.84
1	A	205	SER	N-CA-C	5.83	118.51	110.35
1	F	223	ILE	CB-CA-C	-5.81	101.84	111.32
1	F	291	TYR	CA-C-N	-5.77	112.03	120.75
1	F	291	TYR	C-N-CA	-5.77	112.03	120.75
1	C	100	ALA	N-CA-C	5.73	118.41	109.52
1	D	221	ASP	N-CA-C	-5.73	105.39	112.38
1	E	306	LYS	CB-CA-C	-5.69	110.03	116.63
1	D	267	LYS	N-CA-C	5.67	117.47	111.28
1	F	158	GLY	N-CA-C	5.66	126.60	113.18
1	F	28	ARG	CA-C-N	5.66	125.33	119.56
1	F	28	ARG	C-N-CA	5.66	125.33	119.56
1	E	154	THR	O-C-N	-5.60	116.76	123.31
1	F	291	TYR	N-CA-C	5.58	118.21	111.40
1	A	204	ASN	N-CA-C	5.54	117.32	111.28
1	D	100	ALA	N-CA-C	5.43	118.41	109.72
1	A	305	GLU	N-CA-C	5.37	118.18	109.86
1	B	40	ILE	N-CA-C	5.34	115.55	107.80
1	E	293	VAL	N-CA-C	5.28	117.18	111.58
1	C	154	THR	N-CA-C	5.27	117.40	108.02
1	E	309	LYS	CA-C-N	5.24	127.83	120.28
1	E	309	LYS	C-N-CA	5.24	127.83	120.28
1	D	292	LYS	N-CA-C	5.24	117.07	111.36
1	A	277	TYR	N-CA-C	5.23	119.35	112.92
1	F	31	SER	N-CA-C	-5.21	101.52	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	254	ALA	CB-CA-C	-5.20	110.59	116.63
1	F	264	TYR	N-CA-C	-5.17	106.23	112.54
1	E	162	LEU	CA-C-N	5.17	125.07	119.85
1	E	162	LEU	C-N-CA	5.17	125.07	119.85
1	B	209	GLY	N-CA-C	-5.14	105.96	112.54
1	E	118	ILE	N-CA-C	5.11	114.93	107.37
1	A	254	ALA	CA-C-N	5.07	132.29	121.45
1	A	254	ALA	C-N-CA	5.07	132.29	121.45
1	E	33	ASN	N-CA-C	5.06	117.98	110.14
1	B	24	ILE	N-CA-C	5.06	115.19	108.11
1	A	155	GLY	N-CA-C	5.05	119.86	113.24
1	B	267	LYS	N-CA-C	5.01	116.74	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2210	0	2163	176	0
1	B	2231	0	2205	315	0
1	C	2209	0	2150	177	0
1	D	2248	0	2203	179	0
1	E	2190	0	2154	186	0
1	F	2140	0	2096	167	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
2	C	53	0	31	2	0
2	D	53	0	31	6	0
2	E	53	0	31	3	0
2	F	53	0	31	0	0
3	A	27	0	11	2	0
3	B	27	0	11	3	0
3	C	27	0	11	7	0
3	D	27	0	11	5	0
3	E	27	0	11	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	27	0	11	2	0
4	A	29	0	0	3	0
4	B	29	0	0	4	0
4	C	29	0	0	1	0
4	D	30	0	0	6	0
4	E	22	0	0	2	0
4	F	27	0	0	2	0
All	All	13874	0	13223	1154	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 43.

All (1154) 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:203:ARG:HG3	1:B:204:ASN:CA	1.22	1.61
1:E:122:LYS:HE2	1:E:135:TYR:CE2	1.46	1.45
1:C:200:LEU:HD11	1:C:231:TYR:CE1	1.52	1.42
1:F:256:SER:CB	1:F:257:PHE:HB2	1.51	1.39
1:B:96:LYS:HA	1:B:97:GLN:CB	1.43	1.38
1:A:13:LYS:CE	1:B:95:LYS:HE3	1.54	1.37
1:B:203:ARG:CG	1:B:204:ASN:HA	1.57	1.32
1:C:99:CYS:SG	1:D:99:CYS:HB2	1.67	1.32
1:F:256:SER:OG	1:F:257:PHE:CB	1.77	1.31
1:A:199:ASN:C	1:A:200:LEU:HD12	1.55	1.31
1:C:200:LEU:HD21	1:C:231:TYR:CZ	1.64	1.30
1:D:4:ASN:CB	1:D:5:ASN:HB3	1.60	1.30
1:A:294:MET:CE	1:A:294:MET:HA	1.60	1.29
1:A:296:ILE:HG22	1:A:297:LEU:CD2	1.62	1.29
1:C:200:LEU:O	1:C:200:LEU:CD1	1.79	1.28
1:C:99:CYS:HB2	1:D:99:CYS:SG	1.73	1.27
1:D:306:LYS:N	1:D:307:LYS:HB2	1.47	1.26
1:F:256:SER:OG	1:F:257:PHE:HB2	1.12	1.25
1:E:122:LYS:CE	1:E:135:TYR:HE2	1.51	1.23
1:B:96:LYS:CA	1:B:97:GLN:HB3	1.67	1.23
1:E:97:GLN:N	1:F:99:CYS:HG	1.37	1.23
1:B:203:ARG:CG	1:B:204:ASN:CA	2.12	1.22
1:D:292:LYS:O	1:D:292:LYS:HD3	1.33	1.22
1:B:281:LEU:CD2	1:B:311:VAL:HG13	1.69	1.20
1:B:281:LEU:HD23	1:B:311:VAL:CG1	1.70	1.20
1:B:215:TYR:CE2	1:B:223:ILE:HG23	1.77	1.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:TYR:HE2	1:B:223:ILE:HG23	1.01	1.18
1:E:126:THR:HG22	1:E:127:GLU:C	1.67	1.18
1:F:219:ASN:OD1	1:F:221:ASP:HB2	1.41	1.18
1:F:203:ARG:HH11	1:F:203:ARG:CG	1.57	1.16
1:E:126:THR:HG22	1:E:128:ASN:N	1.59	1.16
1:A:297:LEU:HD23	1:A:297:LEU:N	1.49	1.15
1:D:30:ASN:HB2	1:D:221:ASP:OD2	1.45	1.14
1:A:13:LYS:HE2	1:B:95:LYS:CE	1.75	1.14
1:F:260:GLN:HG2	1:F:292:LYS:HB2	1.14	1.13
1:F:220:GLU:O	1:F:223:ILE:HG13	1.47	1.13
1:D:203:ARG:CG	1:D:204:ASN:HA	1.80	1.11
1:D:249:LYS:C	1:D:250:GLN:OE1	1.94	1.11
1:B:280:GLU:OE1	1:B:310:ARG:HB3	1.49	1.11
1:E:125:GLN:HE21	1:E:127:GLU:HB2	1.11	1.11
1:F:43:ASN:HB2	1:F:45:LEU:HD22	1.24	1.10
1:B:281:LEU:HD23	1:B:311:VAL:HG13	1.13	1.10
1:F:43:ASN:HB2	1:F:45:LEU:CD2	1.81	1.09
1:B:123:TYR:HA	1:B:124:GLU:HB2	1.20	1.09
1:D:4:ASN:HB3	1:D:5:ASN:CB	1.82	1.09
1:A:294:MET:HA	1:A:294:MET:HE2	1.33	1.09
1:D:203:ARG:HG3	1:D:204:ASN:HA	1.09	1.09
1:A:296:ILE:HG22	1:A:297:LEU:HD23	1.13	1.08
1:C:162:LEU:HG	1:C:188:PHE:CD2	1.88	1.08
1:A:13:LYS:CD	1:B:95:LYS:HE3	1.84	1.08
1:B:203:ARG:HD2	1:B:204:ASN:C	1.78	1.07
1:E:305:GLU:HA	1:E:309:LYS:HD2	1.10	1.07
1:C:99:CYS:CB	1:D:99:CYS:SG	2.42	1.06
1:C:166:ALA:O	1:C:167:ILE:HG12	1.52	1.06
1:F:203:ARG:HH11	1:F:203:ARG:HG2	0.94	1.06
1:B:267:LYS:O	1:B:271:LEU:HD12	1.54	1.06
1:E:264:TYR:CD1	1:E:292:LYS:NZ	2.22	1.06
1:B:118:ILE:HD13	1:B:142:ILE:HD13	1.38	1.06
1:C:162:LEU:HG	1:C:188:PHE:CE2	1.91	1.06
1:A:294:MET:HA	1:A:294:MET:HE3	1.39	1.05
1:C:200:LEU:CD1	1:C:231:TYR:CE1	2.40	1.04
1:A:294:MET:HE3	1:A:294:MET:CA	1.83	1.04
1:E:305:GLU:HA	1:E:309:LYS:CD	1.86	1.04
1:F:260:GLN:CG	1:F:292:LYS:HB2	1.87	1.04
1:C:200:LEU:CD1	1:C:231:TYR:HE1	1.69	1.04
1:F:31:SER:HB2	1:F:222:SER:CB	1.87	1.04
1:C:200:LEU:O	1:C:200:LEU:HD13	0.86	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:ARG:HG3	1:B:204:ASN:C	1.84	1.03
1:E:264:TYR:HB2	1:E:292:LYS:CE	1.88	1.02
1:A:97:GLN:NE2	1:A:99:CYS:SG	2.33	1.02
1:E:305:GLU:CA	1:E:309:LYS:HD2	1.89	1.01
1:B:203:ARG:CD	1:B:204:ASN:C	2.33	1.01
1:C:306:LYS:H	1:C:306:LYS:HD2	1.25	1.01
1:C:53:THR:OG1	1:C:157:HIS:HB2	1.58	1.00
1:A:287:LYS:H	1:A:287:LYS:HD3	1.26	1.00
1:B:123:TYR:CA	1:B:124:GLU:HB2	1.87	1.00
1:C:7:ILE:HA	1:C:156:ALA:HB3	1.40	1.00
1:D:60:TYR:CD2	1:D:61:ASN:N	2.29	0.99
1:E:127:GLU:OE1	1:F:308:LYS:HB2	1.63	0.99
1:C:99:CYS:SG	1:D:99:CYS:CB	2.50	0.99
1:C:200:LEU:CD2	1:C:231:TYR:CZ	2.45	0.98
1:F:203:ARG:HG2	1:F:203:ARG:NH1	1.71	0.98
1:B:31:SER:HB2	1:B:222:SER:OG	1.63	0.98
1:C:162:LEU:CG	1:C:188:PHE:CD2	2.46	0.98
1:E:22:ASP:HA	1:E:147:ILE:HD11	1.45	0.98
1:E:290:ARG:O	1:E:291:TYR:HD1	1.46	0.98
1:A:293:VAL:O	1:A:296:ILE:HB	1.65	0.97
1:B:308:LYS:O	1:B:311:VAL:HG23	1.64	0.97
1:A:199:ASN:O	1:A:200:LEU:HD12	1.65	0.97
1:A:13:LYS:HE2	1:B:95:LYS:HE3	0.97	0.96
1:B:203:ARG:CG	1:B:204:ASN:C	2.37	0.96
1:D:57:ILE:O	1:D:58:PRO:O	1.83	0.96
1:E:290:ARG:O	1:E:291:TYR:CD1	2.19	0.96
1:B:35:VAL:HG11	1:B:224:LEU:HD21	1.48	0.96
1:E:40:ILE:HG21	1:E:151:ILE:HD11	1.47	0.96
1:E:281:LEU:HD21	1:E:293:VAL:HG21	1.45	0.96
1:A:294:MET:CE	1:A:294:MET:CA	2.37	0.96
1:E:264:TYR:HB2	1:E:292:LYS:HE3	1.44	0.95
1:C:200:LEU:HD13	1:C:200:LEU:C	1.90	0.95
1:D:6:PHE:O	1:D:9:LEU:HG	1.66	0.95
1:D:4:ASN:N	1:D:5:ASN:C	2.25	0.95
1:F:292:LYS:C	1:F:293:VAL:HG23	1.92	0.95
1:F:45:LEU:N	1:F:45:LEU:CD1	2.30	0.93
1:B:215:TYR:HE2	1:B:223:ILE:CG2	1.83	0.92
1:B:304:ASP:N	1:B:308:LYS:CG	2.33	0.92
1:C:162:LEU:CG	1:C:188:PHE:HD2	1.82	0.92
1:A:13:LYS:CE	1:B:95:LYS:CE	2.40	0.92
1:F:43:ASN:C	1:F:45:LEU:HD13	1.95	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:SER:O	1:A:300:HIS:HB2	1.67	0.91
1:D:305:GLU:C	1:D:307:LYS:HB2	1.93	0.91
1:A:297:LEU:CD2	1:A:297:LEU:N	2.30	0.91
1:B:96:LYS:CA	1:B:97:GLN:CB	2.32	0.91
1:C:42:HIS:CD2	1:C:42:HIS:H	1.85	0.91
1:B:207:TYR:CZ	1:B:209:GLY:HA3	2.06	0.91
2:E:415:FAD:H51A	2:E:415:FAD:H8A	1.49	0.91
1:B:28:ARG:HB2	1:B:221:ASP:OD1	1.70	0.90
1:F:260:GLN:HG2	1:F:292:LYS:CB	1.99	0.90
1:B:118:ILE:HD13	1:B:142:ILE:CD1	2.01	0.90
1:D:304:ASP:N	1:D:307:LYS:HE3	1.87	0.90
1:A:165:ASP:HB2	1:A:169:LYS:HG3	1.50	0.89
1:D:306:LYS:N	1:D:307:LYS:CB	2.35	0.89
1:B:273:LEU:O	1:B:279:CYS:SG	2.30	0.89
1:C:5:ASN:CG	1:C:6:PHE:H	1.81	0.89
1:D:306:LYS:CA	1:D:307:LYS:HB2	2.02	0.89
1:C:200:LEU:HD21	1:C:231:TYR:CE1	2.07	0.88
1:B:287:LYS:HG3	1:B:288:SER:N	1.89	0.88
1:D:203:ARG:HG3	1:D:204:ASN:CA	2.02	0.88
1:F:255:THR:O	1:F:255:THR:HG22	1.70	0.88
2:C:415:FAD:H51A	2:C:415:FAD:H8A	1.53	0.87
1:D:176:ILE:HD12	1:D:283:ILE:HG12	1.56	0.87
1:E:40:ILE:CG2	1:E:151:ILE:HD11	2.04	0.87
1:B:203:ARG:HD2	1:B:204:ASN:O	1.73	0.87
1:B:260:GLN:HE21	1:B:289:ILE:HG12	1.40	0.87
1:D:39:GLU:HB2	4:D:329:HOH:O	1.73	0.87
1:E:264:TYR:CD1	1:E:292:LYS:CE	2.58	0.86
1:E:203:ARG:HG3	1:E:203:ARG:HH11	1.40	0.86
1:B:267:LYS:O	1:B:271:LEU:CD1	2.23	0.86
1:F:296:ILE:HD12	1:F:296:ILE:N	1.89	0.86
1:B:171:THR:O	1:B:207:TYR:CE1	2.28	0.86
1:B:60:TYR:O	1:B:60:TYR:CD2	2.30	0.85
1:B:281:LEU:HB3	1:B:311:VAL:HA	1.59	0.85
1:A:156:ALA:O	1:A:157:HIS:CD2	2.30	0.85
1:C:99:CYS:HG	1:D:99:CYS:HB2	1.34	0.85
1:D:4:ASN:HB3	1:D:5:ASN:HB3	0.85	0.85
1:E:264:TYR:CB	1:E:292:LYS:CE	2.55	0.85
1:E:97:GLN:HB3	1:E:137:TYR:OH	1.75	0.85
2:D:415:FAD:H51A	2:D:415:FAD:H8A	1.56	0.84
1:A:46:PHE:CE1	1:A:154:THR:O	2.30	0.84
1:C:42:HIS:H	1:C:42:HIS:HD2	1.22	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:292:LYS:HD3	1:D:292:LYS:C	1.93	0.84
1:E:203:ARG:HH11	1:E:203:ARG:CG	1.90	0.84
1:F:256:SER:HB2	1:F:257:PHE:HB2	1.58	0.84
1:C:203:ARG:HG3	1:C:203:ARG:HH11	1.41	0.84
1:F:256:SER:CB	1:F:257:PHE:CB	2.47	0.84
1:B:260:GLN:HE22	3:B:416:A2P:H2	1.40	0.84
1:C:42:HIS:O	1:C:43:ASN:HB2	1.78	0.84
1:B:281:LEU:HD23	1:B:311:VAL:CG2	2.08	0.83
1:E:264:TYR:CG	1:E:292:LYS:CE	2.61	0.83
1:C:208:THR:HG22	1:C:208:THR:O	1.76	0.83
1:E:172:ASN:HD22	1:E:277:TYR:HB3	1.41	0.83
1:F:43:ASN:CB	1:F:45:LEU:HD22	2.08	0.83
1:A:253:ASP:HB3	1:B:264:TYR:OH	1.76	0.83
1:D:6:PHE:CD1	1:D:47:LYS:HB3	2.12	0.83
1:B:296:ILE:CG2	1:B:296:ILE:O	2.26	0.83
1:C:53:THR:OG1	1:C:157:HIS:CB	2.25	0.83
1:D:296:ILE:O	1:D:296:ILE:HG22	1.79	0.83
1:B:94:ILE:HG22	1:B:95:LYS:N	1.93	0.83
1:F:292:LYS:O	1:F:293:VAL:HG23	1.78	0.83
1:B:296:ILE:O	1:B:297:LEU:HD12	1.78	0.83
1:E:122:LYS:CE	1:E:135:TYR:CE2	2.38	0.83
1:B:134:ASN:HD22	1:B:135:TYR:H	1.23	0.82
1:F:261:ASP:HA	1:F:292:LYS:CE	2.09	0.82
1:B:96:LYS:HA	1:B:97:GLN:HB2	1.60	0.82
1:C:199:ASN:OD1	1:C:201:TYR:CE2	2.32	0.82
1:F:261:ASP:HA	1:F:292:LYS:HE2	1.60	0.82
1:A:118:ILE:HD13	1:A:142:ILE:HG13	1.59	0.82
1:A:196:ASP:O	1:A:200:LEU:HD11	1.79	0.82
1:E:308:LYS:H	1:E:308:LYS:HD2	1.43	0.81
1:A:156:ALA:O	1:A:157:HIS:CG	2.32	0.81
1:E:118:ILE:HG21	1:E:142:ILE:HG13	1.61	0.81
1:D:182:ILE:HD11	1:D:224:LEU:HB2	1.62	0.81
1:A:196:ASP:O	1:A:200:LEU:CD1	2.29	0.81
1:E:264:TYR:CB	1:E:292:LYS:HE2	2.09	0.81
1:A:13:LYS:HD3	1:B:95:LYS:CE	2.11	0.81
1:D:251:ASN:O	1:D:252:SER:OG	1.98	0.81
1:E:125:GLN:NE2	1:E:127:GLU:HB2	1.94	0.81
1:E:126:THR:HG21	1:E:128:ASN:HB3	1.61	0.81
1:C:178:THR:CG2	1:C:289:ILE:HD11	2.11	0.80
1:B:147:ILE:HD12	1:B:147:ILE:N	1.94	0.80
1:C:162:LEU:CD1	1:C:188:PHE:HD2	1.94	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:PRO:HG2	1:F:166:ALA:HB2	1.63	0.80
1:D:46:PHE:CE1	1:D:154:THR:O	2.33	0.80
1:B:171:THR:O	1:B:207:TYR:HE1	1.63	0.80
1:E:99:CYS:SG	1:F:99:CYS:CB	2.70	0.80
1:B:132:ILE:HG23	1:B:132:ILE:O	1.81	0.80
1:B:266:ARG:HD2	1:B:269:GLU:CB	2.12	0.80
1:E:264:TYR:HB2	1:E:292:LYS:HE2	1.60	0.80
1:D:249:LYS:O	1:D:250:GLN:OE1	2.00	0.79
1:D:252:SER:HG	1:D:255:THR:N	1.78	0.79
1:F:31:SER:HB2	1:F:222:SER:OG	1.81	0.79
1:A:13:LYS:CD	1:B:95:LYS:CE	2.61	0.79
1:A:167:ILE:HD12	1:A:167:ILE:N	1.97	0.79
1:B:177:ALA:HB2	1:B:185:TYR:HE1	1.47	0.79
1:C:166:ALA:O	1:C:167:ILE:CG1	2.30	0.79
1:F:271:LEU:HD11	1:F:299:SER:HB2	1.64	0.79
1:F:296:ILE:N	1:F:296:ILE:CD1	2.45	0.79
1:D:4:ASN:CB	1:D:5:ASN:CB	2.49	0.79
1:E:28:ARG:HB3	1:E:29:PRO:HD2	1.63	0.79
1:B:188:PHE:O	1:B:192:LEU:HD13	1.82	0.79
1:E:57:ILE:HG12	1:E:100:ALA:HB2	1.63	0.79
1:E:97:GLN:N	1:F:99:CYS:SG	2.54	0.79
1:A:10:TYR:H	1:A:155:GLY:HA3	1.46	0.79
1:F:31:SER:HB2	1:F:222:SER:HB3	1.64	0.79
1:F:45:LEU:HD13	1:F:45:LEU:H	1.48	0.79
1:B:94:ILE:HG22	1:B:95:LYS:H	1.46	0.78
1:C:306:LYS:H	1:C:306:LYS:CD	1.95	0.78
1:B:304:ASP:O	1:B:305:GLU:HB3	1.83	0.78
1:F:175:PHE:HB2	1:F:213:ILE:HG12	1.65	0.78
1:D:12:VAL:CG1	1:D:98:ARG:HD3	2.13	0.78
1:F:45:LEU:N	1:F:45:LEU:HD13	1.97	0.78
1:C:305:GLU:HG2	1:C:308:LYS:HE3	1.64	0.78
1:D:307:LYS:CG	4:D:338:HOH:O	2.32	0.78
1:C:162:LEU:CD2	1:C:188:PHE:CD2	2.67	0.78
1:D:101:ARG:HG3	2:D:415:FAD:H4'	1.65	0.78
1:D:203:ARG:HE	1:D:204:ASN:C	1.91	0.78
1:B:260:GLN:HE22	3:B:416:A2P:C2	1.95	0.78
1:F:248:TYR:O	1:F:248:TYR:CD1	2.37	0.78
1:D:4:ASN:N	1:D:5:ASN:O	2.17	0.78
1:B:281:LEU:HD23	1:B:311:VAL:HG22	1.66	0.77
1:E:122:LYS:HE2	1:E:135:TYR:CD2	2.19	0.77
1:A:267:LYS:HG3	1:A:296:ILE:CD1	2.13	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:LEU:HD23	1:B:311:VAL:CB	2.14	0.77
1:E:242:ILE:HD11	1:E:244:TYR:CE2	2.20	0.77
1:F:219:ASN:HB3	1:F:222:SER:OG	1.84	0.77
1:A:296:ILE:CG2	1:A:297:LEU:CD2	2.55	0.77
1:E:290:ARG:O	1:E:291:TYR:HB2	1.84	0.77
1:D:46:PHE:CZ	1:D:154:THR:O	2.38	0.77
1:A:199:ASN:C	1:A:200:LEU:CD1	2.49	0.76
1:B:280:GLU:OE2	1:B:310:ARG:HD2	1.84	0.76
1:B:296:ILE:O	1:B:296:ILE:HG22	1.84	0.76
1:D:234:LYS:O	1:D:237:PRO:HD3	1.85	0.76
1:B:296:ILE:C	1:B:297:LEU:HD12	2.10	0.76
1:C:162:LEU:HD21	1:C:188:PHE:CD2	2.20	0.76
1:E:264:TYR:O	1:E:267:LYS:HG2	1.85	0.76
1:D:251:ASN:O	1:D:252:SER:CB	2.34	0.76
1:C:257:PHE:HE2	1:C:262:GLU:HG2	1.51	0.75
1:E:126:THR:CG2	1:E:127:GLU:C	2.53	0.75
1:E:127:GLU:OE1	1:F:308:LYS:CB	2.32	0.75
1:F:219:ASN:OD1	1:F:221:ASP:CB	2.30	0.75
1:C:10:TYR:HB2	1:C:155:GLY:H	1.51	0.75
1:C:272:ASN:OD1	1:C:272:ASN:N	2.18	0.75
1:D:61:ASN:CG	1:D:61:ASN:O	2.30	0.75
1:E:126:THR:CG2	1:E:128:ASN:N	2.46	0.75
1:E:281:LEU:CD2	1:E:293:VAL:HG21	2.16	0.75
1:B:296:ILE:C	1:B:297:LEU:CD1	2.60	0.75
1:F:256:SER:OG	1:F:257:PHE:HB3	1.81	0.75
1:A:5:ASN:C	1:A:5:ASN:HD22	1.94	0.75
1:B:96:LYS:HA	1:B:97:GLN:HB3	0.77	0.75
1:C:5:ASN:O	1:C:6:PHE:HB2	1.85	0.74
1:F:43:ASN:CB	1:F:45:LEU:CD2	2.65	0.74
1:A:296:ILE:CG2	1:A:297:LEU:HD23	2.05	0.74
1:F:178:THR:HB	3:F:416:A2P:H5'1	1.69	0.74
1:D:125:GLN:HE21	1:D:132:ILE:HG12	1.52	0.74
1:B:110:ASN:ND2	1:B:111:MET:HG3	2.03	0.74
1:C:305:GLU:HA	1:C:307:LYS:H	1.52	0.74
1:E:280:GLU:OE2	1:E:310:ARG:HG2	1.88	0.74
1:F:293:VAL:HA	1:F:296:ILE:HD13	1.69	0.74
1:B:134:ASN:HD22	1:B:135:TYR:N	1.84	0.74
1:A:299:SER:O	1:A:300:HIS:CB	2.34	0.74
1:B:147:ILE:H	1:B:147:ILE:CD1	2.01	0.74
1:F:203:ARG:CG	1:F:203:ARG:NH1	2.30	0.74
1:B:165:ASP:HA	1:E:203:ARG:HE	1.50	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:HG12	1:D:98:ARG:HD3	1.69	0.73
1:E:26:LEU:HG	1:E:37:HIS:HB2	1.70	0.73
1:E:243:HIS:H	1:E:243:HIS:CD2	2.04	0.73
1:C:260:GLN:OE1	3:C:416:A2P:H2	1.87	0.73
1:D:307:LYS:HG2	4:D:338:HOH:O	1.88	0.73
1:B:110:ASN:C	1:B:110:ASN:HD22	1.94	0.73
1:E:308:LYS:HD2	1:E:308:LYS:N	2.02	0.73
1:F:45:LEU:N	1:F:45:LEU:HD12	2.02	0.73
1:B:309:LYS:O	1:B:310:ARG:HB2	1.89	0.73
1:F:260:GLN:OE1	1:F:292:LYS:N	2.21	0.73
1:E:290:ARG:O	1:E:291:TYR:CB	2.35	0.73
1:D:292:LYS:HA	1:D:292:LYS:HE3	1.68	0.73
1:D:260:GLN:NE2	3:D:416:A2P:H2	2.03	0.73
1:C:257:PHE:CE2	1:C:262:GLU:HG2	2.23	0.72
1:B:297:LEU:CD1	1:B:297:LEU:N	2.51	0.72
1:D:182:ILE:HD11	1:D:224:LEU:CB	2.19	0.72
1:A:167:ILE:HD12	1:A:167:ILE:H	1.52	0.72
1:A:296:ILE:HG22	1:A:297:LEU:HD21	1.70	0.72
1:D:123:TYR:CE1	1:D:134:ASN:HB2	2.23	0.72
1:E:264:TYR:CD1	1:E:292:LYS:HE3	2.24	0.72
1:B:298:LYS:O	1:B:298:LYS:CD	2.37	0.72
1:E:122:LYS:HE2	1:E:135:TYR:HE2	0.66	0.72
1:B:177:ALA:HB2	1:B:185:TYR:CE1	2.24	0.72
1:E:177:ALA:HB2	1:E:185:TYR:HE2	1.52	0.72
1:A:294:MET:HE3	1:A:294:MET:N	2.05	0.72
1:B:165:ASP:HA	1:E:203:ARG:NE	2.04	0.72
1:C:162:LEU:HD11	1:C:188:PHE:HD2	1.55	0.72
1:C:42:HIS:CD2	1:C:42:HIS:N	2.58	0.72
1:C:178:THR:HG23	1:C:289:ILE:HD11	1.72	0.72
1:F:248:TYR:CD1	1:F:248:TYR:C	2.62	0.71
1:B:304:ASP:N	1:B:308:LYS:HD2	2.05	0.71
1:B:223:ILE:HD13	1:B:244:TYR:CD2	2.25	0.71
1:A:296:ILE:C	1:A:297:LEU:HD23	2.13	0.71
1:B:28:ARG:HB3	1:B:29:PRO:CD	2.21	0.71
1:C:98:ARG:HA	1:C:98:ARG:NE	2.04	0.71
1:C:184:PRO:O	1:C:188:PHE:CD1	2.43	0.71
1:C:304:ASP:CB	1:C:307:LYS:HE2	2.21	0.71
1:B:280:GLU:OE1	1:B:310:ARG:CB	2.36	0.71
1:B:304:ASP:N	1:B:308:LYS:HG2	2.03	0.71
1:B:223:ILE:HD13	1:B:244:TYR:CE2	2.26	0.71
1:D:203:ARG:CB	1:D:204:ASN:HA	2.20	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:308:LYS:H	1:E:308:LYS:CD	2.04	0.71
1:B:27:VAL:HB	1:B:31:SER:OG	1.91	0.70
1:B:147:ILE:N	1:B:147:ILE:CD1	2.54	0.70
1:B:194:ALA:HB3	1:B:204:ASN:HB3	1.74	0.70
1:E:264:TYR:CB	1:E:292:LYS:HE3	2.19	0.70
1:B:298:LYS:O	1:B:298:LYS:HD3	1.90	0.70
1:D:35:VAL:HG11	1:D:224:LEU:HD21	1.72	0.70
1:B:202:ASN:CB	1:B:203:ARG:HA	2.21	0.70
1:B:298:LYS:H	1:B:298:LYS:HD2	1.57	0.70
1:C:200:LEU:HD21	1:C:231:TYR:CE2	2.24	0.70
1:E:293:VAL:O	1:E:297:LEU:HD23	1.90	0.70
1:A:10:TYR:HB2	1:A:155:GLY:N	2.07	0.70
1:A:165:ASP:HB2	1:A:169:LYS:CG	2.21	0.70
1:C:177:ALA:HB2	1:C:185:TYR:HE2	1.55	0.70
1:F:27:VAL:HG21	1:F:33:ASN:O	1.92	0.70
1:B:155:GLY:O	1:B:157:HIS:CD2	2.44	0.70
1:C:102:LEU:HD21	1:C:157:HIS:CE1	2.26	0.70
1:B:4:ASN:O	1:B:6:PHE:N	2.22	0.69
1:C:304:ASP:HB2	1:C:307:LYS:HE2	1.72	0.69
1:A:253:ASP:HA	1:B:264:TYR:CZ	2.27	0.69
1:B:10:TYR:O	1:B:155:GLY:N	2.24	0.69
1:C:166:ALA:O	1:C:167:ILE:HG23	1.91	0.69
1:B:305:GLU:O	1:B:305:GLU:HG3	1.92	0.69
1:C:101:ARG:HH21	1:C:137:TYR:HB3	1.58	0.69
1:F:291:TYR:O	1:F:292:LYS:C	2.30	0.69
1:E:22:ASP:HA	1:E:147:ILE:CD1	2.23	0.69
1:F:43:ASN:HB2	1:F:45:LEU:CD1	2.22	0.69
1:A:267:LYS:HG3	1:A:296:ILE:HD13	1.74	0.69
1:D:57:ILE:C	1:D:58:PRO:O	2.36	0.69
1:F:174:ILE:HD11	1:F:214:TYR:HE1	1.56	0.69
1:B:30:ASN:O	1:B:219:ASN:ND2	2.26	0.69
1:B:203:ARG:CD	1:B:204:ASN:CA	2.70	0.69
1:B:203:ARG:H	1:B:204:ASN:HA	1.57	0.69
1:B:266:ARG:HD2	1:B:269:GLU:HB3	1.74	0.69
1:C:5:ASN:CG	1:C:6:PHE:N	2.50	0.69
1:C:5:ASN:O	1:C:6:PHE:CB	2.41	0.68
1:E:280:GLU:CD	1:E:310:ARG:HB3	2.18	0.68
1:C:177:ALA:HB2	1:C:185:TYR:CE2	2.29	0.68
1:B:273:LEU:C	1:B:279:CYS:HG	2.00	0.68
1:F:292:LYS:O	1:F:293:VAL:CG2	2.42	0.68
1:A:200:LEU:HD12	1:A:200:LEU:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:ILE:HG21	1:E:151:ILE:CD1	2.23	0.68
1:B:304:ASP:O	1:B:305:GLU:CB	2.41	0.67
1:D:60:TYR:HD2	1:D:61:ASN:N	1.86	0.67
1:E:188:PHE:O	1:E:192:LEU:HG	1.94	0.67
1:B:60:TYR:O	1:B:60:TYR:CG	2.47	0.67
1:B:271:LEU:O	1:B:275:ASN:ND2	2.27	0.67
1:C:166:ALA:C	1:C:167:ILE:HG23	2.19	0.67
1:F:165:ASP:O	1:F:169:LYS:HB2	1.94	0.67
1:C:98:ARG:HA	1:C:98:ARG:HE	1.58	0.67
1:C:264:TYR:O	1:C:267:LYS:HB2	1.95	0.67
1:F:296:ILE:CD1	1:F:296:ILE:H	2.06	0.67
1:E:99:CYS:SG	1:F:99:CYS:HB2	2.34	0.67
1:F:292:LYS:O	1:F:293:VAL:CB	2.43	0.67
1:B:3:GLU:HG2	1:B:4:ASN:HB3	1.75	0.67
1:A:292:LYS:O	1:A:292:LYS:HG2	1.95	0.67
1:E:243:HIS:H	1:E:243:HIS:HD2	1.43	0.67
1:B:273:LEU:C	1:B:279:CYS:SG	2.78	0.66
1:F:28:ARG:NH1	1:F:226:LEU:HG	2.10	0.66
1:F:50:GLU:OE2	1:F:109:ASN:HB2	1.95	0.66
1:F:174:ILE:HG23	1:F:281:LEU:HA	1.76	0.66
1:D:14:ASN:ND2	1:D:14:ASN:O	2.29	0.66
1:F:293:VAL:CA	1:F:296:ILE:HD13	2.25	0.66
1:E:167:ILE:HG22	1:E:167:ILE:O	1.93	0.66
1:F:10:TYR:HB2	1:F:155:GLY:H	1.60	0.66
1:D:304:ASP:N	1:D:307:LYS:HG3	2.10	0.66
1:B:281:LEU:CD2	1:B:311:VAL:HG22	2.26	0.66
1:F:255:THR:O	1:F:255:THR:CG2	2.44	0.66
1:C:162:LEU:HG	1:C:188:PHE:HE2	1.55	0.66
1:D:307:LYS:CE	4:D:338:HOH:O	2.44	0.66
1:B:304:ASP:N	1:B:308:LYS:CD	2.59	0.66
1:E:122:LYS:HG2	1:E:135:TYR:CD2	2.31	0.66
1:F:199:ASN:HD22	1:F:199:ASN:N	1.94	0.66
1:F:248:TYR:O	1:F:248:TYR:HD1	1.79	0.66
1:E:38:LEU:HB2	1:E:116:VAL:HG12	1.78	0.66
1:A:290:ARG:O	1:A:294:MET:HB2	1.96	0.65
1:B:131:ASN:HB2	1:B:133:THR:HG22	1.78	0.65
1:B:30:ASN:HB2	1:B:221:ASP:CG	2.21	0.65
1:B:266:ARG:HG3	1:B:266:ARG:O	1.96	0.65
1:B:309:LYS:O	1:B:310:ARG:CB	2.43	0.65
1:A:13:LYS:HB3	1:B:95:LYS:CE	2.27	0.65
1:B:172:ASN:HD22	1:B:277:TYR:HB3	1.62	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASN:ND2	4:B:342:HOH:O	2.30	0.65
1:D:60:TYR:CD2	1:D:60:TYR:C	2.75	0.65
1:F:219:ASN:OD1	1:F:221:ASP:N	2.29	0.65
1:A:167:ILE:H	1:A:167:ILE:CD1	2.08	0.65
1:F:244:TYR:HB3	1:F:246:PHE:CE2	2.31	0.65
1:A:13:LYS:HD3	1:B:95:LYS:HE3	1.68	0.65
1:B:203:ARG:HG3	1:B:204:ASN:HA	0.66	0.65
1:B:218:TYR:HA	1:B:247:SER:HB2	1.77	0.65
1:C:203:ARG:HG3	1:C:203:ARG:NH1	2.05	0.65
1:E:97:GLN:HB3	1:E:137:TYR:CZ	2.32	0.65
1:E:243:HIS:CD2	1:E:243:HIS:N	2.65	0.65
1:E:18:CYS:HB2	1:E:151:ILE:HD12	1.79	0.64
1:F:281:LEU:HB3	1:F:310:ARG:O	1.97	0.64
1:C:200:LEU:CD2	1:C:231:TYR:CE1	2.79	0.64
1:D:292:LYS:HA	1:D:292:LYS:CE	2.25	0.64
1:E:290:ARG:C	1:E:291:TYR:CD1	2.74	0.64
1:F:172:ASN:HD22	1:F:277:TYR:HB3	1.61	0.64
1:A:13:LYS:HB3	1:B:95:LYS:HE3	1.78	0.64
1:B:260:GLN:NE2	3:B:416:A2P:H2	2.12	0.64
2:C:415:FAD:H51A	2:C:415:FAD:C8A	2.26	0.64
1:A:231:TYR:CZ	1:A:235:MET:HG3	2.33	0.64
1:C:102:LEU:HD21	1:C:157:HIS:ND1	2.13	0.64
1:C:208:THR:O	1:C:208:THR:CG2	2.44	0.64
1:E:126:THR:HG21	1:E:128:ASN:CB	2.28	0.64
1:A:57:ILE:HG22	1:A:60:TYR:HB2	1.78	0.64
1:A:200:LEU:HB3	1:A:231:TYR:OH	1.97	0.64
1:E:310:ARG:O	1:E:312:HIS:CD2	2.50	0.64
1:A:57:ILE:CG2	1:A:60:TYR:HB2	2.28	0.63
1:B:287:LYS:CG	1:B:288:SER:N	2.62	0.63
1:F:258:TYR:HB3	3:F:416:A2P:C2	2.29	0.63
1:B:308:LYS:O	1:B:311:VAL:CG2	2.44	0.63
1:B:219:ASN:OD1	1:B:222:SER:HB2	1.97	0.63
1:E:118:ILE:HD12	1:E:142:ILE:CD1	2.29	0.63
1:A:177:ALA:HB2	1:A:185:TYR:CE2	2.34	0.63
1:D:260:GLN:HG2	1:D:289:ILE:HA	1.81	0.63
1:C:167:ILE:HG22	1:C:192:LEU:CD2	2.29	0.63
1:C:200:LEU:CD2	1:C:231:TYR:OH	2.46	0.63
1:B:131:ASN:N	1:B:131:ASN:OD1	2.32	0.62
1:B:297:LEU:N	1:B:297:LEU:HD13	2.14	0.62
1:C:200:LEU:CD1	1:C:200:LEU:C	2.62	0.62
1:A:208:THR:HA	1:A:239:ASN:HD21	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ILE:HG22	1:C:192:LEU:HD23	1.81	0.62
1:C:184:PRO:O	1:C:188:PHE:HD1	1.80	0.62
1:F:31:SER:CB	1:F:222:SER:HB3	2.29	0.62
1:B:281:LEU:CD2	1:B:311:VAL:CG1	2.49	0.62
1:E:127:GLU:O	1:E:128:ASN:C	2.43	0.62
1:E:177:ALA:HB2	1:E:185:TYR:CE2	2.33	0.62
1:F:261:ASP:CA	1:F:292:LYS:HE2	2.29	0.62
1:D:58:PRO:HG2	1:D:137:TYR:CE2	2.34	0.62
1:F:43:ASN:HB2	1:F:45:LEU:HD13	1.79	0.62
1:A:97:GLN:HE21	1:A:99:CYS:CB	2.13	0.62
1:C:273:LEU:O	1:C:279:CYS:SG	2.52	0.62
1:E:260:GLN:NE2	3:E:416:A2P:N1	2.48	0.62
1:A:293:VAL:O	1:A:296:ILE:CB	2.45	0.62
1:B:264:TYR:O	1:B:267:LYS:HG2	1.99	0.62
1:D:46:PHE:HE1	1:D:154:THR:O	1.83	0.62
1:A:172:ASN:HB3	1:A:279:CYS:SG	2.40	0.62
1:B:304:ASP:HA	1:B:308:LYS:HD2	1.81	0.62
1:C:30:ASN:HB2	1:C:221:ASP:OD2	2.00	0.62
1:D:226:LEU:HD22	1:D:230:GLU:HG3	1.82	0.62
1:E:57:ILE:HD11	1:E:154:THR:HG21	1.81	0.62
1:B:158:GLY:HA3	4:B:318:HOH:O	2.00	0.62
1:A:37:HIS:CE1	1:A:115:SER:HB2	2.35	0.61
1:B:123:TYR:CB	1:B:124:GLU:HB2	2.29	0.61
1:D:304:ASP:N	1:D:307:LYS:CE	2.61	0.61
1:B:207:TYR:CE2	1:B:209:GLY:CA	2.83	0.61
1:D:305:GLU:N	1:D:307:LYS:HG3	2.16	0.61
1:A:13:LYS:HE2	1:B:95:LYS:CD	2.30	0.61
1:B:266:ARG:CD	1:B:269:GLU:CB	2.79	0.61
1:F:43:ASN:CB	1:F:45:LEU:HD13	2.30	0.61
1:B:146:LYS:O	1:B:149:ASP:HB2	2.00	0.61
1:A:271:LEU:HD13	1:A:300:HIS:HB2	1.83	0.61
1:E:101:ARG:HH21	1:E:137:TYR:HB3	1.64	0.61
2:B:415:FAD:O5B	2:B:415:FAD:H8A	1.99	0.61
1:B:101:ARG:NH1	1:B:137:TYR:HD2	1.99	0.61
1:A:167:ILE:N	1:A:167:ILE:CD1	2.64	0.61
1:D:177:ALA:HA	1:D:284:CYS:O	2.01	0.61
1:C:54:CYS:HA	1:C:157:HIS:HD2	1.65	0.60
1:E:98:ARG:HB2	1:F:97:GLN:HA	1.83	0.60
1:E:197:LYS:HD2	4:E:336:HOH:O	2.01	0.60
1:B:94:ILE:O	1:B:95:LYS:HG2	2.01	0.60
1:C:97:GLN:O	1:C:98:ARG:HB2	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:LYS:CA	1:D:307:LYS:CB	2.73	0.60
1:A:196:ASP:O	1:A:200:LEU:HD12	2.01	0.60
1:B:298:LYS:HD2	1:B:298:LYS:N	2.16	0.60
1:C:102:LEU:HD22	1:C:157:HIS:CG	2.36	0.60
1:C:305:GLU:HA	1:C:307:LYS:N	2.16	0.60
1:C:306:LYS:HD2	1:C:306:LYS:N	2.05	0.60
1:F:292:LYS:C	1:F:293:VAL:CG2	2.63	0.60
1:B:147:ILE:HD12	1:B:147:ILE:H	1.62	0.60
1:B:207:TYR:O	1:B:209:GLY:N	2.34	0.60
1:A:253:ASP:CB	1:B:264:TYR:OH	2.49	0.60
1:B:43:ASN:HD22	1:C:206:ASN:HD21	1.49	0.60
1:E:255:THR:HG22	1:F:256:SER:H	1.67	0.60
1:B:43:ASN:HD22	1:C:206:ASN:ND2	2.00	0.60
1:F:293:VAL:C	1:F:296:ILE:HD13	2.26	0.60
1:C:5:ASN:O	1:C:6:PHE:CD1	2.55	0.60
1:C:304:ASP:HB3	1:C:307:LYS:HD3	1.82	0.60
1:E:126:THR:CG2	1:E:128:ASN:CB	2.79	0.60
1:F:256:SER:CA	1:F:257:PHE:HB2	2.30	0.60
1:C:245:VAL:HG22	1:C:262:GLU:HG3	1.84	0.60
1:E:50:GLU:CD	1:E:191:LYS:HD2	2.27	0.60
1:A:97:GLN:NE2	1:A:99:CYS:CB	2.64	0.60
1:B:180:THR:HA	1:B:224:LEU:HD12	1.84	0.60
1:A:10:TYR:HD1	1:A:155:GLY:HA2	1.68	0.59
1:B:192:LEU:CD1	1:B:192:LEU:N	2.65	0.59
1:D:203:ARG:NE	1:D:204:ASN:O	2.34	0.59
1:B:296:ILE:HG22	1:B:297:LEU:CD1	2.32	0.59
1:E:264:TYR:CG	1:E:292:LYS:HE2	2.36	0.59
1:F:174:ILE:HD11	1:F:214:TYR:CE1	2.37	0.59
1:B:19:LYS:HD2	1:B:148:ASN:HD22	1.66	0.59
1:A:46:PHE:HE1	1:A:154:THR:O	1.83	0.59
1:B:97:GLN:O	1:B:97:GLN:HG2	2.02	0.59
1:D:4:ASN:CG	1:D:5:ASN:HB3	2.25	0.59
1:D:250:GLN:HA	1:D:251:ASN:C	2.27	0.59
1:E:18:CYS:HB2	1:E:151:ILE:CD1	2.32	0.59
1:E:203:ARG:HG2	1:E:235:MET:HE1	1.85	0.59
1:F:9:LEU:HD13	1:F:47:LYS:HG3	1.83	0.59
1:E:99:CYS:CB	1:F:99:CYS:SG	2.91	0.59
1:F:174:ILE:CD1	1:F:214:TYR:HE1	2.14	0.59
1:B:304:ASP:CA	1:B:308:LYS:HD2	2.32	0.59
1:E:264:TYR:CG	1:E:292:LYS:NZ	2.70	0.59
1:B:133:THR:OG1	1:B:134:ASN:N	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLY:N	1:D:154:THR:OG1	2.36	0.59
1:D:246:PHE:O	1:D:248:TYR:N	2.36	0.59
1:F:173:PHE:HB2	1:F:211:ILE:HG12	1.85	0.59
1:A:298:LYS:O	1:A:299:SER:OG	2.17	0.59
1:D:266:ARG:NH1	1:D:269:GLU:HG2	2.18	0.59
1:A:13:LYS:HE2	1:B:95:LYS:HG3	1.85	0.59
1:B:281:LEU:CG	1:B:311:VAL:HG13	2.32	0.59
1:D:5:ASN:C	1:D:5:ASN:HD22	2.08	0.59
1:D:177:ALA:HB2	1:D:185:TYR:HE1	1.68	0.59
1:B:19:LYS:HD2	1:B:148:ASN:ND2	2.17	0.58
1:B:134:ASN:ND2	4:B:335:HOH:O	2.30	0.58
1:B:203:ARG:N	1:B:204:ASN:HA	2.14	0.58
1:E:280:GLU:OE2	1:E:310:ARG:CG	2.50	0.58
1:C:196:ASP:HB3	1:C:199:ASN:O	2.03	0.58
1:B:284:CYS:HA	1:B:314:GLU:O	2.04	0.58
1:E:123:TYR:CE1	1:E:134:ASN:HB3	2.38	0.58
1:A:297:LEU:HD23	1:A:297:LEU:H	1.63	0.58
1:A:257:PHE:CE2	1:A:262:GLU:HG2	2.39	0.58
1:B:5:ASN:O	1:B:5:ASN:ND2	2.34	0.58
1:E:98:ARG:O	1:F:97:GLN:NE2	2.37	0.58
1:D:4:ASN:OD1	1:D:4:ASN:C	2.46	0.58
1:A:55:GLY:N	1:A:154:THR:OG1	2.37	0.58
1:B:269:GLU:OE1	1:B:269:GLU:O	2.22	0.58
1:A:280:GLU:OE1	1:A:310:ARG:HA	2.04	0.57
1:B:31:SER:CB	1:B:222:SER:OG	2.47	0.57
1:E:182:ILE:CG2	1:E:183:SER:N	2.67	0.57
1:B:207:TYR:CZ	1:B:209:GLY:CA	2.82	0.57
1:D:123:TYR:CE1	1:D:134:ASN:CB	2.86	0.57
1:F:57:ILE:HG12	1:F:100:ALA:HB2	1.85	0.57
1:A:257:PHE:HE2	1:A:262:GLU:HG2	1.70	0.57
1:D:177:ALA:HB2	1:D:185:TYR:CE1	2.40	0.57
1:F:244:TYR:CB	1:F:246:PHE:CE2	2.87	0.57
1:A:5:ASN:C	1:A:5:ASN:ND2	2.62	0.57
1:B:171:THR:O	1:B:207:TYR:OH	2.21	0.57
1:B:298:LYS:O	1:B:298:LYS:HD2	2.03	0.57
1:D:123:TYR:O	1:D:124:GLU:HB2	2.04	0.57
1:F:43:ASN:CB	1:F:45:LEU:CD1	2.82	0.57
1:B:35:VAL:CG1	1:B:224:LEU:HD21	2.30	0.57
1:E:258:TYR:HB2	1:E:260:GLN:OE1	2.05	0.57
1:F:261:ASP:HA	1:F:292:LYS:HE3	1.85	0.57
1:B:266:ARG:CD	1:B:269:GLU:HB3	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:28:ARG:HB3	1:D:29:PRO:CD	2.35	0.57
1:E:123:TYR:O	1:E:134:ASN:HB2	2.04	0.57
1:B:165:ASP:HB3	1:E:203:ARG:NH2	2.19	0.57
1:E:203:ARG:HG3	1:E:203:ARG:NH1	2.17	0.57
1:B:304:ASP:N	1:B:308:LYS:HG3	2.18	0.57
1:D:132:ILE:O	1:D:132:ILE:HG13	2.05	0.57
1:D:252:SER:OG	1:D:255:THR:N	2.38	0.57
1:B:56:ILE:O	1:B:58:PRO:HD3	2.05	0.57
1:B:290:ARG:NH2	1:B:313:VAL:HG11	2.19	0.57
1:F:293:VAL:HA	1:F:296:ILE:CD1	2.35	0.57
1:B:217:VAL:HG21	1:B:223:ILE:HG12	1.87	0.56
1:B:271:LEU:O	1:B:272:ASN:C	2.47	0.56
1:C:200:LEU:CG	1:C:231:TYR:CE1	2.87	0.56
1:B:207:TYR:C	1:B:209:GLY:H	2.13	0.56
1:C:58:PRO:O	1:C:59:TYR:HB2	2.06	0.56
1:B:49:LEU:O	1:B:50:GLU:C	2.48	0.56
1:B:123:TYR:HA	1:B:124:GLU:CB	2.14	0.56
1:B:296:ILE:C	1:B:297:LEU:HD13	2.28	0.56
1:C:167:ILE:CG2	1:C:192:LEU:HD23	2.34	0.56
1:D:207:TYR:CZ	1:D:209:GLY:HA3	2.40	0.56
1:E:288:SER:CB	3:E:416:A2P:HN62	2.19	0.56
1:A:177:ALA:HB2	1:A:185:TYR:HE2	1.70	0.56
1:B:203:ARG:CD	1:B:204:ASN:O	2.45	0.56
1:C:53:THR:HG22	1:C:104:SER:HA	1.85	0.56
1:B:171:THR:O	1:B:207:TYR:CZ	2.58	0.56
1:E:118:ILE:HD12	1:E:142:ILE:HD12	1.86	0.56
1:D:231:TYR:CZ	1:D:235:MET:HG3	2.41	0.56
1:D:260:GLN:HE21	3:D:416:A2P:H2	1.71	0.56
1:E:172:ASN:ND2	1:E:277:TYR:HB3	2.17	0.56
1:C:165:ASP:O	1:C:168:GLN:N	2.37	0.56
1:B:202:ASN:HB3	1:B:203:ARG:HA	1.88	0.56
1:C:297:LEU:HD12	1:C:297:LEU:N	2.21	0.56
1:E:162:LEU:HG	1:E:188:PHE:CE2	2.41	0.56
1:F:111:MET:HE1	1:F:190:LYS:HD3	1.87	0.56
1:E:290:ARG:O	1:E:291:TYR:CG	2.59	0.56
1:B:94:ILE:CG2	1:B:95:LYS:H	2.06	0.55
1:B:298:LYS:CD	1:B:298:LYS:C	2.79	0.55
1:E:126:THR:HG22	1:E:127:GLU:CA	2.35	0.55
1:B:207:TYR:CE2	1:B:209:GLY:C	2.84	0.55
1:D:60:TYR:CD2	1:D:61:ASN:CA	2.89	0.55
1:D:307:LYS:HE2	4:D:338:HOH:O	2.03	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:292:LYS:O	1:F:293:VAL:HB	2.06	0.55
1:A:97:GLN:HB2	1:A:99:CYS:SG	2.45	0.55
1:B:203:ARG:CG	1:B:204:ASN:N	2.60	0.55
1:B:280:GLU:CD	1:B:310:ARG:HD2	2.31	0.55
1:A:162:LEU:HG	1:A:188:PHE:CD2	2.41	0.55
1:B:270:PHE:C	1:B:270:PHE:CD2	2.85	0.55
1:E:62:GLU:O	1:E:62:GLU:HG2	2.06	0.55
1:E:178:THR:HG23	1:E:289:ILE:HD11	1.88	0.55
1:A:279:CYS:O	1:A:310:ARG:NH1	2.39	0.55
1:B:10:TYR:H	1:B:155:GLY:HA3	1.72	0.55
1:C:98:ARG:NE	1:C:98:ARG:CA	2.69	0.55
1:D:260:GLN:NE2	3:D:416:A2P:C2	2.69	0.55
1:B:43:ASN:CB	1:C:206:ASN:HD21	2.20	0.55
1:C:181:GLY:O	1:C:184:PRO:HD2	2.07	0.55
1:F:26:LEU:HB2	1:F:35:VAL:CG2	2.36	0.55
1:B:231:TYR:CZ	1:B:235:MET:HG3	2.42	0.55
1:D:50:GLU:CD	1:D:191:LYS:HD2	2.32	0.55
1:A:97:GLN:HG3	1:A:137:TYR:OH	2.07	0.54
1:B:28:ARG:HB3	1:B:29:PRO:HD2	1.88	0.54
1:B:203:ARG:HD3	1:B:204:ASN:N	2.22	0.54
1:F:37:HIS:CE1	1:F:115:SER:HB2	2.43	0.54
1:D:203:ARG:NH1	1:D:204:ASN:O	2.40	0.54
1:D:304:ASP:N	1:D:307:LYS:CD	2.70	0.54
1:F:32:PRO:C	1:F:33:ASN:OD1	2.50	0.54
1:B:10:TYR:HB2	1:B:155:GLY:N	2.21	0.54
1:B:53:THR:OG1	1:B:102:LEU:HB3	2.08	0.54
1:B:118:ILE:CD1	1:B:142:ILE:HD13	2.25	0.54
1:C:200:LEU:HD22	1:C:231:TYR:OH	2.07	0.54
1:A:293:VAL:C	1:A:296:ILE:HB	2.30	0.54
1:B:41:ASN:HA	1:B:113:ASN:OD1	2.07	0.54
1:C:37:HIS:CE1	1:C:115:SER:HB2	2.43	0.54
1:C:305:GLU:HB3	1:C:306:LYS:HA	1.89	0.54
1:E:174:ILE:HD11	1:E:273:LEU:HB3	1.90	0.54
2:E:415:FAD:H51A	2:E:415:FAD:C8A	2.30	0.54
1:A:267:LYS:HE3	1:A:296:ILE:HD13	1.90	0.54
1:D:27:VAL:HG13	1:D:35:VAL:HG13	1.89	0.54
1:D:215:TYR:CE1	1:D:217:VAL:HG13	2.42	0.54
1:F:140:GLY:O	1:F:144:ASN:ND2	2.41	0.54
1:A:260:GLN:OE1	3:A:416:A2P:H2	2.08	0.54
1:B:305:GLU:O	1:B:305:GLU:CG	2.56	0.54
1:C:272:ASN:O	1:C:276:ASN:N	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD13	1:B:192:LEU:H	1.73	0.54
1:C:200:LEU:HD11	1:C:231:TYR:HE1	0.72	0.54
1:D:4:ASN:CG	1:D:5:ASN:CB	2.80	0.54
1:D:53:THR:CG2	1:D:157:HIS:HB2	2.37	0.54
1:A:97:GLN:HG3	1:A:137:TYR:CZ	2.43	0.53
1:F:43:ASN:HB2	1:F:45:LEU:CG	2.37	0.53
1:F:160:PHE:O	1:F:160:PHE:CD2	2.61	0.53
1:A:292:LYS:O	1:A:292:LYS:CG	2.56	0.53
1:D:5:ASN:C	1:D:5:ASN:ND2	2.62	0.53
1:D:14:ASN:O	1:D:14:ASN:CG	2.51	0.53
1:E:20:ILE:HD13	1:E:40:ILE:HG12	1.89	0.53
1:F:296:ILE:HG22	1:F:296:ILE:O	2.08	0.53
1:B:190:LYS:O	1:B:193:PHE:O	2.27	0.53
1:A:114:LEU:C	1:A:114:LEU:HD12	2.34	0.53
1:B:110:ASN:HD22	1:B:111:MET:HG3	1.71	0.53
1:B:297:LEU:HD23	1:B:308:LYS:NZ	2.23	0.53
1:F:10:TYR:HB2	1:F:155:GLY:N	2.23	0.53
1:F:101:ARG:NH1	1:F:137:TYR:HD2	2.06	0.53
1:B:101:ARG:CG	2:B:415:FAD:H4'	2.38	0.53
1:A:13:LYS:HE2	1:B:95:LYS:CG	2.38	0.53
1:A:266:ARG:NH2	4:A:339:HOH:O	2.38	0.53
1:B:164:ASN:O	1:E:203:ARG:HD2	2.08	0.53
1:C:306:LYS:C	1:C:308:LYS:H	2.14	0.53
1:F:176:ILE:HD12	1:F:283:ILE:HG12	1.90	0.53
1:F:291:TYR:C	1:F:292:LYS:O	2.44	0.53
1:A:46:PHE:CZ	1:A:154:THR:O	2.61	0.53
1:D:6:PHE:O	1:D:7:ILE:C	2.52	0.53
1:E:127:GLU:CD	1:F:308:LYS:HB2	2.33	0.53
1:F:101:ARG:NH1	1:F:137:TYR:CD2	2.77	0.53
1:B:203:ARG:CD	1:B:204:ASN:N	2.72	0.53
1:B:273:LEU:HB3	1:B:279:CYS:SG	2.49	0.53
1:C:166:ALA:O	1:C:167:ILE:CG2	2.57	0.53
3:C:416:A2P:OP1	1:D:287:LYS:HE2	2.08	0.53
1:D:4:ASN:CA	1:D:5:ASN:HB3	2.37	0.53
1:D:296:ILE:O	1:D:296:ILE:CG2	2.51	0.53
1:B:178:THR:HG23	1:B:289:ILE:HD11	1.91	0.52
1:D:39:GLU:OE2	1:D:113:ASN:ND2	2.42	0.52
1:D:46:PHE:HZ	1:D:154:THR:O	1.92	0.52
1:F:160:PHE:O	1:F:160:PHE:CG	2.62	0.52
1:A:162:LEU:HG	1:A:188:PHE:CE2	2.44	0.52
3:C:416:A2P:OP1	1:D:287:LYS:NZ	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ASP:C	1:D:307:LYS:HG3	2.34	0.52
1:E:182:ILE:HG23	1:E:183:SER:N	2.23	0.52
1:F:60:TYR:HB3	1:F:152:TYR:CD1	2.44	0.52
1:A:200:LEU:CD1	1:A:200:LEU:N	2.72	0.52
1:C:165:ASP:O	1:C:168:GLN:HB2	2.09	0.52
1:A:291:TYR:O	1:A:295:ASP:N	2.33	0.52
1:A:296:ILE:HG22	1:A:297:LEU:N	2.22	0.52
1:C:301:ASP:OD1	1:C:304:ASP:OD2	2.28	0.52
1:F:28:ARG:HB3	1:F:29:PRO:HD2	1.92	0.52
1:C:247:SER:HG	3:C:416:A2P:HO3'	1.52	0.52
1:A:25:ASN:OD1	1:A:27:VAL:HG22	2.09	0.52
1:A:30:ASN:HB2	1:A:221:ASP:CG	2.35	0.52
1:C:272:ASN:O	1:C:273:LEU:C	2.53	0.52
1:F:249:LYS:HB3	4:F:328:HOH:O	2.10	0.52
1:A:11:THR:OG1	1:A:13:LYS:HG2	2.10	0.52
1:A:193:PHE:CD1	1:A:236:TYR:CD2	2.97	0.52
1:B:203:ARG:N	1:B:204:ASN:CA	2.72	0.52
1:B:218:TYR:HD2	1:B:219:ASN:CG	2.18	0.52
1:E:280:GLU:OE2	1:E:310:ARG:HB3	2.10	0.52
1:E:286:LEU:O	1:E:289:ILE:HG13	2.09	0.52
1:A:291:TYR:O	1:A:295:ASP:HB2	2.09	0.51
1:E:255:THR:CG2	1:F:256:SER:H	2.22	0.51
1:B:296:ILE:O	1:B:296:ILE:HG23	2.10	0.51
1:C:165:ASP:HB2	1:C:169:LYS:HG3	1.91	0.51
1:D:122:LYS:HG2	1:D:135:TYR:HE2	1.75	0.51
1:D:145:LEU:HD11	1:D:151:ILE:HD12	1.92	0.51
1:E:28:ARG:CB	1:E:29:PRO:HD2	2.38	0.51
1:E:203:ARG:CG	1:E:203:ARG:NH1	2.61	0.51
1:E:264:TYR:CG	1:E:292:LYS:HE3	2.41	0.51
1:F:6:PHE:HB3	1:F:47:LYS:HB2	1.91	0.51
1:B:298:LYS:HD3	1:B:298:LYS:C	2.35	0.51
2:D:415:FAD:H51A	2:D:415:FAD:C8A	2.33	0.51
1:D:4:ASN:ND2	1:D:5:ASN:HB2	2.26	0.51
1:C:41:ASN:HA	1:C:113:ASN:OD1	2.10	0.51
1:C:166:ALA:O	1:C:167:ILE:CB	2.59	0.51
1:D:10:TYR:O	1:D:155:GLY:N	2.33	0.51
1:D:123:TYR:CZ	1:D:134:ASN:HB3	2.44	0.51
1:B:290:ARG:CZ	1:B:313:VAL:HG11	2.39	0.51
1:E:13:LYS:O	1:E:15:PRO:HD3	2.09	0.51
1:A:176:ILE:HD12	1:A:283:ILE:HG12	1.92	0.51
1:B:217:VAL:CG2	1:B:223:ILE:HG12	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:PHE:O	1:C:9:LEU:HG	2.11	0.51
1:C:176:ILE:HD13	1:C:263:ILE:HD13	1.92	0.51
1:A:96:LYS:C	1:A:96:LYS:HD2	2.36	0.51
1:C:55:GLY:O	1:C:153:LEU:HA	2.10	0.51
1:A:97:GLN:NE2	1:A:99:CYS:HB2	2.25	0.51
1:D:37:HIS:CE1	1:D:115:SER:HB2	2.46	0.51
1:A:223:ILE:HD13	1:A:244:TYR:CE2	2.46	0.51
1:F:31:SER:HB2	1:F:222:SER:CA	2.38	0.51
1:A:288:SER:O	1:A:289:ILE:C	2.52	0.50
1:B:203:ARG:CG	1:B:205:SER:N	2.73	0.50
1:D:196:ASP:HB3	1:D:199:ASN:HB2	1.92	0.50
1:E:11:THR:HG23	1:E:14:ASN:H	1.74	0.50
1:F:294:MET:CG	1:F:295:ASP:N	2.74	0.50
1:A:178:THR:HG23	1:A:289:ILE:HD11	1.94	0.50
1:B:3:GLU:HG2	1:B:4:ASN:CA	2.41	0.50
1:B:226:LEU:HD22	1:B:230:GLU:HG3	1.94	0.50
1:F:7:ILE:HD13	1:F:159:TYR:CE2	2.46	0.50
1:A:53:THR:OG1	1:A:157:HIS:HB2	2.11	0.50
1:A:196:ASP:O	1:A:199:ASN:O	2.29	0.50
1:B:277:TYR:CD1	1:B:277:TYR:N	2.79	0.50
1:D:218:TYR:HA	1:D:247:SER:HB3	1.93	0.50
1:E:40:ILE:HG23	1:E:151:ILE:HD11	1.91	0.50
1:A:5:ASN:ND2	1:A:5:ASN:O	2.32	0.50
1:B:28:ARG:CB	1:B:221:ASP:OD1	2.53	0.50
1:C:5:ASN:N	4:C:323:HOH:O	2.44	0.50
1:B:10:TYR:HB2	1:B:155:GLY:H	1.76	0.50
1:C:305:GLU:CB	1:C:306:LYS:HA	2.42	0.50
1:E:167:ILE:O	1:E:167:ILE:CG2	2.58	0.50
1:B:26:LEU:HD12	1:B:224:LEU:HD22	1.93	0.50
1:C:25:ASN:OD1	1:C:27:VAL:HG22	2.12	0.50
1:C:304:ASP:HB3	1:C:307:LYS:CD	2.41	0.50
1:C:162:LEU:CG	1:C:188:PHE:CE2	2.78	0.50
1:D:61:ASN:O	1:D:61:ASN:OD1	2.30	0.50
1:D:250:GLN:OE1	1:D:250:GLN:N	2.41	0.50
1:D:118:ILE:HD13	1:D:142:ILE:HG13	1.94	0.50
1:E:204:ASN:OD1	1:E:204:ASN:O	2.30	0.50
1:A:17:LYS:HG3	1:A:152:TYR:CZ	2.47	0.50
1:A:196:ASP:O	1:A:197:LYS:C	2.55	0.50
1:E:293:VAL:O	1:E:297:LEU:HB2	2.11	0.50
1:A:156:ALA:C	1:A:157:HIS:CD2	2.90	0.49
1:A:101:ARG:HH21	1:A:137:TYR:HB3	1.76	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ARG:HG2	2:B:415:FAD:H4'	1.92	0.49
1:B:159:TYR:C	1:B:161:ASN:H	2.21	0.49
1:D:123:TYR:HD1	1:D:124:GLU:HG3	1.77	0.49
1:F:24:ILE:HA	4:F:318:HOH:O	2.13	0.49
1:F:135:TYR:CE2	1:F:143:LYS:HG3	2.48	0.49
1:F:231:TYR:CZ	1:F:235:MET:HG3	2.47	0.49
1:F:290:ARG:HG2	1:F:313:VAL:HG21	1.94	0.49
1:D:5:ASN:O	1:D:5:ASN:ND2	2.46	0.49
1:D:97:GLN:HG3	1:D:97:GLN:O	2.12	0.49
1:B:43:ASN:HB2	1:C:206:ASN:HD21	1.77	0.49
1:B:203:ARG:N	1:B:204:ASN:CG	2.70	0.49
1:A:156:ALA:C	1:A:157:HIS:CG	2.91	0.49
1:B:214:TYR:CE2	1:B:243:HIS:CD2	3.00	0.49
1:B:266:ARG:CD	1:B:269:GLU:HB2	2.42	0.49
1:E:127:GLU:O	1:E:128:ASN:O	2.30	0.49
1:F:218:TYR:CD1	1:F:248:TYR:HB2	2.48	0.49
1:D:60:TYR:CD2	1:D:61:ASN:HA	2.48	0.49
1:E:220:GLU:C	1:E:222:SER:H	2.20	0.49
1:B:261:ASP:OD2	1:B:292:LYS:HE2	2.13	0.49
1:F:43:ASN:C	1:F:45:LEU:CD1	2.76	0.49
1:A:60:TYR:CD2	1:A:61:ASN:HB2	2.48	0.49
1:C:180:THR:HA	1:C:224:LEU:HD12	1.95	0.49
1:F:260:GLN:CD	1:F:292:LYS:HB2	2.38	0.49
1:A:56:ILE:O	1:A:100:ALA:HA	2.13	0.49
1:A:105:ILE:HG22	1:A:107:SER:H	1.77	0.49
1:B:6:PHE:O	1:B:9:LEU:HD13	2.13	0.49
1:B:174:ILE:HD11	1:B:273:LEU:HB3	1.93	0.49
1:A:138:CYS:HB3	2:A:415:FAD:O1P	2.13	0.48
1:B:60:TYR:O	1:B:61:ASN:OD1	2.30	0.48
1:B:114:LEU:HD12	1:B:114:LEU:C	2.38	0.48
1:E:114:LEU:HD12	1:E:114:LEU:O	2.13	0.48
1:A:13:LYS:CB	1:B:95:LYS:NZ	2.76	0.48
1:B:172:ASN:HA	1:B:207:TYR:OH	2.13	0.48
1:E:42:HIS:C	1:E:43:ASN:HD22	2.21	0.48
1:E:138:CYS:O	1:E:142:ILE:HG12	2.13	0.48
1:F:33:ASN:OD1	1:F:33:ASN:N	2.46	0.48
1:E:24:ILE:HB	1:E:37:HIS:HB3	1.94	0.48
1:E:204:ASN:O	1:E:204:ASN:CG	2.56	0.48
1:C:20:ILE:HD13	1:C:151:ILE:HD11	1.95	0.48
1:C:203:ARG:O	1:C:204:ASN:C	2.56	0.48
1:E:215:TYR:HE2	1:E:223:ILE:HG23	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:GLU:HG3	1:A:306:LYS:N	2.28	0.48
1:B:3:GLU:HG2	1:B:4:ASN:CB	2.41	0.48
1:B:174:ILE:HG13	1:B:279:CYS:HB3	1.95	0.48
1:E:172:ASN:HB3	1:E:279:CYS:SG	2.54	0.48
1:E:310:ARG:O	1:E:312:HIS:HD2	1.94	0.48
1:F:231:TYR:CE1	1:F:235:MET:HG3	2.48	0.48
1:B:4:ASN:C	1:B:6:PHE:H	2.16	0.48
1:B:148:ASN:ND2	1:B:148:ASN:O	2.46	0.48
1:B:313:VAL:HG13	1:B:313:VAL:O	2.13	0.48
1:D:122:LYS:HG2	1:D:135:TYR:CE2	2.48	0.48
1:F:244:TYR:HB3	1:F:246:PHE:CZ	2.49	0.48
1:F:296:ILE:HD13	1:F:296:ILE:H	1.77	0.48
1:C:102:LEU:CD2	1:C:157:HIS:CG	2.96	0.48
1:F:287:LYS:CG	1:F:288:SER:N	2.75	0.48
1:B:280:GLU:CD	1:B:310:ARG:HB3	2.33	0.48
1:D:60:TYR:HD2	1:D:60:TYR:C	2.19	0.48
1:F:220:GLU:HA	1:F:246:PHE:CE1	2.49	0.48
1:A:257:PHE:HA	1:A:261:ASP:OD2	2.13	0.47
1:B:160:PHE:CG	1:B:314:GLU:OE1	2.67	0.47
1:C:297:LEU:HD12	1:C:297:LEU:H	1.78	0.47
1:D:114:LEU:HD12	1:D:114:LEU:C	2.39	0.47
1:B:162:LEU:HG	1:B:188:PHE:CE2	2.50	0.47
1:D:204:ASN:OD1	1:D:204:ASN:N	2.47	0.47
1:D:220:GLU:HG3	1:D:246:PHE:CZ	2.49	0.47
1:D:104:SER:HB2	1:D:183:SER:CB	2.44	0.47
1:D:304:ASP:N	1:D:307:LYS:CG	2.77	0.47
1:B:170:ASN:OD1	1:E:238:ASN:ND2	2.40	0.47
1:A:155:GLY:O	1:A:156:ALA:CB	2.62	0.47
1:C:301:ASP:OD2	1:C:304:ASP:N	2.47	0.47
1:E:310:ARG:H	1:E:310:ARG:HD3	1.78	0.47
1:B:207:TYR:CE2	1:B:209:GLY:O	2.67	0.47
1:B:215:TYR:CE2	1:B:223:ILE:CG2	2.67	0.47
1:A:199:ASN:O	1:A:200:LEU:CD1	2.52	0.47
1:B:228:GLU:OE2	1:B:228:GLU:N	2.45	0.47
1:B:305:GLU:O	1:B:306:LYS:HB2	2.14	0.47
1:C:5:ASN:OD1	1:C:6:PHE:N	2.43	0.47
1:C:101:ARG:HH21	1:C:137:TYR:HD2	1.62	0.47
1:C:304:ASP:HB2	1:C:307:LYS:CE	2.44	0.47
1:E:119:LYS:HD3	4:E:322:HOH:O	2.14	0.47
1:E:126:THR:HG22	1:E:127:GLU:N	2.29	0.47
1:B:46:PHE:CE2	1:B:48:TYR:HB3	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:HB3	1:B:152:TYR:CD1	2.50	0.47
1:B:162:LEU:HG	1:B:188:PHE:CD2	2.49	0.47
1:E:281:LEU:HB3	1:E:311:VAL:HG22	1.97	0.47
1:C:53:THR:OG1	1:C:157:HIS:HB3	2.13	0.47
1:A:206:ASN:N	1:A:206:ASN:HD22	2.13	0.46
1:A:249:LYS:HG3	1:A:249:LYS:O	2.14	0.46
1:B:208:THR:HA	1:B:239:ASN:ND2	2.30	0.46
1:C:300:HIS:O	1:C:301:ASP:C	2.58	0.46
1:D:57:ILE:HG13	1:D:100:ALA:HB2	1.97	0.46
1:E:174:ILE:HD12	1:E:279:CYS:SG	2.54	0.46
1:C:304:ASP:HB3	1:C:307:LYS:HE2	1.95	0.46
1:F:233:GLN:O	1:F:233:GLN:HG2	2.15	0.46
1:B:178:THR:O	1:B:179:GLY:C	2.58	0.46
1:F:262:GLU:O	1:F:265:LYS:CB	2.63	0.46
1:B:95:LYS:O	1:B:97:GLN:HB2	2.14	0.46
1:B:110:ASN:HD22	1:B:111:MET:N	2.13	0.46
1:D:125:GLN:OE1	1:D:125:GLN:HA	2.16	0.46
1:A:55:GLY:O	1:A:153:LEU:HA	2.15	0.46
1:A:204:ASN:N	1:A:204:ASN:HD22	2.12	0.46
1:D:104:SER:HB2	1:D:183:SER:HB3	1.96	0.46
1:B:94:ILE:O	1:B:95:LYS:CG	2.64	0.46
1:C:102:LEU:CD2	1:C:157:HIS:ND1	2.78	0.46
1:D:182:ILE:HG12	1:D:215:TYR:CE2	2.51	0.46
1:C:292:LYS:NZ	1:D:250:GLN:HB2	2.31	0.46
1:F:255:THR:O	1:F:256:SER:HB3	2.15	0.46
1:A:182:ILE:HD13	1:A:215:TYR:CD2	2.50	0.46
1:C:97:GLN:O	1:C:98:ARG:CB	2.64	0.46
1:E:126:THR:CB	1:F:290:ARG:HH22	2.28	0.46
1:E:167:ILE:O	1:E:170:ASN:ND2	2.49	0.46
1:D:110:ASN:N	1:D:110:ASN:OD1	2.48	0.46
1:D:260:GLN:CG	1:D:289:ILE:HA	2.46	0.46
1:D:306:LYS:HA	1:D:307:LYS:HB2	1.90	0.46
1:F:107:SER:OG	1:F:114:LEU:HA	2.16	0.46
1:F:262:GLU:O	1:F:265:LYS:HB3	2.15	0.46
1:A:28:ARG:HB3	1:A:29:PRO:HD2	1.98	0.46
1:B:290:ARG:NH2	1:B:313:VAL:CG1	2.79	0.46
1:F:27:VAL:HG23	1:F:27:VAL:O	2.15	0.46
1:F:220:GLU:O	1:F:223:ILE:CG1	2.40	0.45
1:B:203:ARG:H	1:B:204:ASN:CA	2.27	0.45
1:B:208:THR:HA	1:B:239:ASN:HD21	1.82	0.45
1:C:176:ILE:HD13	1:C:263:ILE:CD1	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:416:A2P:OP1	1:D:287:LYS:CE	2.65	0.45
1:F:174:ILE:CD1	1:F:214:TYR:CE1	2.96	0.45
1:F:22:ASP:HA	1:F:147:ILE:HD11	1.96	0.45
1:A:155:GLY:O	1:A:156:ALA:HB2	2.16	0.45
1:A:253:ASP:CA	1:B:264:TYR:OH	2.65	0.45
1:A:288:SER:O	1:A:290:ARG:N	2.49	0.45
1:A:291:TYR:O	1:A:295:ASP:CB	2.65	0.45
1:B:4:ASN:C	1:B:6:PHE:N	2.73	0.45
1:D:4:ASN:N	1:D:5:ASN:CA	2.80	0.45
1:D:216:GLY:O	3:D:416:A2P:H4'	2.16	0.45
1:D:260:GLN:HE22	3:D:416:A2P:C2	2.28	0.45
1:B:248:TYR:CD2	1:B:248:TYR:C	2.93	0.45
1:D:175:PHE:HB3	1:D:185:TYR:CD1	2.51	0.45
1:F:43:ASN:CA	1:F:45:LEU:HD13	2.47	0.45
1:A:10:TYR:H	1:A:155:GLY:CA	2.25	0.45
1:C:304:ASP:CB	1:C:307:LYS:CE	2.92	0.45
1:E:281:LEU:CD2	1:E:293:VAL:CG2	2.92	0.45
1:E:292:LYS:O	1:E:296:ILE:HB	2.17	0.45
1:E:307:LYS:O	1:E:308:LYS:C	2.60	0.45
1:A:23:LYS:HE2	1:A:36:TYR:CD2	2.51	0.45
1:A:297:LEU:HD22	1:A:297:LEU:HA	1.65	0.45
1:B:260:GLN:NE2	1:B:289:ILE:HG12	2.20	0.45
1:B:310:ARG:HD3	4:B:336:HOH:O	2.15	0.45
1:F:182:ILE:O	1:F:183:SER:C	2.59	0.45
1:A:165:ASP:O	1:A:165:ASP:OD2	2.33	0.45
1:A:287:LYS:HD3	1:A:287:LYS:N	2.10	0.45
1:B:169:LYS:HB3	1:B:171:THR:HG23	1.99	0.45
1:D:229:LEU:O	1:D:233:GLN:HB2	2.17	0.45
1:D:180:THR:HA	1:D:224:LEU:HD12	1.99	0.45
1:D:189:LEU:HD22	1:D:193:PHE:HE2	1.81	0.45
1:B:266:ARG:O	1:B:266:ARG:CG	2.64	0.45
1:D:28:ARG:HB3	1:D:29:PRO:HD2	1.99	0.45
1:D:53:THR:HG22	1:D:157:HIS:HB2	1.98	0.45
1:D:248:TYR:HA	1:D:249:LYS:HA	1.68	0.45
1:F:263:ILE:HG23	1:F:270:PHE:CD1	2.52	0.45
1:C:199:ASN:OD1	1:C:201:TYR:CD2	2.68	0.44
1:D:123:TYR:CZ	1:D:134:ASN:CB	3.00	0.44
1:E:175:PHE:HB2	1:E:213:ILE:HG12	1.99	0.44
1:E:179:GLY:O	1:E:224:LEU:HD12	2.18	0.44
1:B:38:LEU:HB2	1:B:116:VAL:HG12	1.99	0.44
1:E:42:HIS:O	1:E:43:ASN:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:235:MET:C	1:E:237:PRO:HD3	2.42	0.44
1:F:271:LEU:O	1:F:275:ASN:N	2.44	0.44
1:A:13:LYS:CB	1:B:95:LYS:HE3	2.46	0.44
1:C:247:SER:OG	3:C:416:A2P:O3'	2.28	0.44
1:C:306:LYS:HG2	1:C:306:LYS:O	2.17	0.44
1:D:306:LYS:HA	1:D:308:LYS:N	2.32	0.44
1:C:178:THR:HG21	1:C:289:ILE:HD11	1.98	0.44
1:C:182:ILE:HD13	1:C:215:TYR:CG	2.53	0.44
1:D:7:ILE:HA	1:D:156:ALA:O	2.17	0.44
1:D:249:LYS:O	1:D:249:LYS:HG3	2.18	0.44
1:F:154:THR:O	1:F:157:HIS:NE2	2.50	0.44
1:F:160:PHE:CE2	1:F:282:TYR:HD2	2.36	0.44
1:A:13:LYS:HB3	1:B:95:LYS:NZ	2.32	0.44
1:B:3:GLU:HA	1:B:4:ASN:HA	1.59	0.44
1:B:182:ILE:HB	1:B:215:TYR:CE1	2.52	0.44
1:C:6:PHE:CE1	1:C:49:LEU:HD13	2.51	0.44
1:B:202:ASN:O	1:B:204:ASN:ND2	2.50	0.44
1:B:220:GLU:CD	1:B:220:GLU:H	2.25	0.44
1:B:304:ASP:O	1:B:304:ASP:OD1	2.35	0.44
1:C:5:ASN:O	1:C:6:PHE:CG	2.70	0.44
1:E:203:ARG:HG2	1:E:235:MET:CE	2.47	0.44
1:C:305:GLU:CG	1:C:308:LYS:HE3	2.41	0.44
1:D:53:THR:HG23	1:D:102:LEU:HD22	2.00	0.44
1:D:125:GLN:NE2	1:D:132:ILE:HG12	2.29	0.44
1:E:49:LEU:O	1:E:52:HIS:HB2	2.17	0.44
1:A:34:GLU:O	1:A:120:ILE:HG12	2.18	0.44
1:B:110:ASN:HD21	1:B:111:MET:HG3	1.82	0.44
1:B:242:ILE:HG21	1:B:244:TYR:CZ	2.53	0.44
1:C:114:LEU:C	1:C:114:LEU:HD12	2.43	0.44
1:E:160:PHE:CZ	1:E:284:CYS:HB2	2.53	0.44
1:F:31:SER:HA	1:F:32:PRO:HD3	1.50	0.44
1:A:42:HIS:O	1:A:43:ASN:HB2	2.18	0.43
1:A:170:ASN:HB2	4:A:325:HOH:O	2.17	0.43
1:B:26:LEU:CD1	1:B:224:LEU:HD22	2.48	0.43
1:B:96:LYS:CB	1:B:97:GLN:HB3	2.39	0.43
1:B:192:LEU:N	1:B:192:LEU:HD12	2.33	0.43
1:B:233:GLN:HA	1:B:240:ILE:CG2	2.48	0.43
1:C:46:PHE:HZ	1:C:154:THR:C	2.25	0.43
1:C:162:LEU:HD11	1:C:188:PHE:CD2	2.44	0.43
1:D:182:ILE:HD11	1:D:224:LEU:HB3	1.97	0.43
1:E:260:GLN:HG2	1:E:289:ILE:HA	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:415:FAD:O5B	2:E:415:FAD:O5'	2.36	0.43
1:B:176:ILE:HD12	1:B:283:ILE:HG12	1.99	0.43
1:B:214:TYR:CE2	1:B:243:HIS:HD2	2.36	0.43
1:C:102:LEU:CD2	1:C:157:HIS:CE1	2.99	0.43
1:D:207:TYR:HE2	1:D:209:GLY:O	2.01	0.43
1:E:99:CYS:HB2	1:F:99:CYS:SG	2.58	0.43
1:A:267:LYS:CG	1:A:296:ILE:CD1	2.93	0.43
1:A:306:LYS:HA	1:A:306:LYS:HD3	1.61	0.43
1:B:26:LEU:HD13	1:B:224:LEU:HB3	2.00	0.43
1:B:207:TYR:C	1:B:209:GLY:N	2.74	0.43
1:C:101:ARG:NH2	1:C:137:TYR:CD2	2.87	0.43
1:D:49:LEU:O	1:D:52:HIS:HB2	2.18	0.43
1:F:295:ASP:O	1:F:297:LEU:N	2.45	0.43
1:A:111:MET:HE1	1:A:190:LYS:HD3	2.01	0.43
1:A:296:ILE:CG2	1:A:297:LEU:HD21	2.39	0.43
1:B:14:ASN:O	1:B:14:ASN:CG	2.61	0.43
1:B:26:LEU:HD23	1:B:26:LEU:HA	1.81	0.43
1:B:186:ILE:HG22	1:B:190:LYS:HE3	2.00	0.43
1:C:167:ILE:CG2	1:C:192:LEU:CD2	2.94	0.43
1:A:293:VAL:O	1:A:296:ILE:N	2.51	0.43
1:B:43:ASN:HD22	1:C:206:ASN:CG	2.25	0.43
1:B:101:ARG:NH1	1:B:137:TYR:CD2	2.84	0.43
1:D:220:GLU:C	1:D:222:SER:N	2.75	0.43
1:D:306:LYS:N	1:D:307:LYS:CG	2.81	0.43
1:E:126:THR:HB	1:F:290:ARG:NH2	2.32	0.43
1:F:101:ARG:HH11	1:F:137:TYR:HD2	1.66	0.43
1:A:17:LYS:HG3	1:A:152:TYR:CE2	2.53	0.43
1:A:253:ASP:O	1:A:253:ASP:OD1	2.37	0.43
1:B:165:ASP:CB	1:E:203:ARG:HH21	2.30	0.43
1:C:203:ARG:NH1	1:C:203:ARG:CG	2.75	0.43
1:C:265:LYS:C	1:C:267:LYS:H	2.26	0.43
1:F:31:SER:CB	1:F:222:SER:CB	2.76	0.43
1:A:36:TYR:HE2	4:A:318:HOH:O	2.02	0.43
1:A:260:GLN:NE2	3:A:416:A2P:N1	2.59	0.43
1:B:269:GLU:OE1	1:B:269:GLU:C	2.62	0.43
1:C:31:SER:HA	1:C:32:PRO:HD3	1.92	0.43
1:E:118:ILE:HB	1:E:142:ILE:HG21	2.01	0.43
1:E:164:ASN:OD1	1:E:164:ASN:N	2.28	0.43
1:A:31:SER:HB2	1:A:222:SER:OG	2.18	0.43
1:C:20:ILE:HG12	1:C:151:ILE:HG12	2.00	0.43
1:D:4:ASN:ND2	1:D:5:ASN:CB	2.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:PRO:HB2	1:D:152:TYR:HB3	2.01	0.43
1:F:260:GLN:CD	1:F:288:SER:O	2.61	0.43
1:B:266:ARG:HD2	1:B:269:GLU:HB2	1.96	0.43
1:C:16:LEU:HD23	1:C:46:PHE:CD1	2.54	0.43
1:D:281:LEU:HD23	1:D:282:TYR:N	2.33	0.43
1:E:170:ASN:N	1:E:170:ASN:HD22	2.15	0.43
1:A:13:LYS:HD3	1:B:95:LYS:HZ1	1.84	0.43
1:C:292:LYS:O	1:C:292:LYS:HG3	2.19	0.43
1:F:14:ASN:CG	1:F:14:ASN:O	2.62	0.43
1:F:145:LEU:HD23	1:F:145:LEU:HA	1.89	0.43
1:A:28:ARG:HB3	1:A:29:PRO:CD	2.49	0.42
1:C:293:VAL:O	1:C:297:LEU:CD1	2.67	0.42
1:C:306:LYS:CD	1:C:306:LYS:N	2.69	0.42
1:A:151:ILE:O	1:A:151:ILE:HG23	2.19	0.42
1:A:298:LYS:HD2	1:A:304:ASP:OD1	2.20	0.42
1:B:111:MET:O	1:B:112:GLU:C	2.62	0.42
1:B:281:LEU:HD21	1:B:311:VAL:HG13	1.86	0.42
1:C:275:ASN:OD1	1:C:307:LYS:NZ	2.52	0.42
1:D:105:ILE:HG22	1:D:107:SER:H	1.83	0.42
1:E:24:ILE:CG2	1:E:25:ASN:N	2.81	0.42
1:E:281:LEU:HB3	1:E:311:VAL:HG13	2.00	0.42
1:E:285:GLY:H	1:E:315:VAL:HG12	1.84	0.42
1:F:287:LYS:HG3	1:F:288:SER:N	2.29	0.42
1:A:250:GLN:OE1	1:A:250:GLN:HA	2.19	0.42
1:B:123:TYR:HB2	1:B:124:GLU:C	2.44	0.42
1:B:305:GLU:C	1:B:307:LYS:N	2.73	0.42
1:C:172:ASN:O	1:C:279:CYS:HA	2.20	0.42
1:C:264:TYR:HD1	1:C:296:ILE:HD11	1.84	0.42
2:A:415:FAD:H1'1	2:A:415:FAD:H9	1.76	0.42
1:B:189:LEU:HD13	1:B:232:PHE:CD1	2.55	0.42
1:E:155:GLY:HA3	1:E:156:ALA:HA	1.90	0.42
1:E:165:ASP:HA	1:E:168:GLN:OE1	2.20	0.42
1:E:294:MET:HA	1:E:297:LEU:HB2	2.00	0.42
1:F:158:GLY:O	1:F:159:TYR:HB2	2.18	0.42
1:A:13:LYS:HD3	1:B:95:LYS:NZ	2.33	0.42
1:B:100:ALA:C	1:B:101:ARG:HD2	2.44	0.42
1:B:172:ASN:HA	1:B:207:TYR:HH	1.84	0.42
1:C:260:GLN:OE1	3:C:416:A2P:C2	2.65	0.42
1:E:264:TYR:CE1	1:E:292:LYS:NZ	2.66	0.42
1:E:264:TYR:HD1	1:E:292:LYS:HE3	1.80	0.42
1:F:43:ASN:O	1:F:45:LEU:CD1	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:CYS:N	2:A:415:FAD:O1P	2.49	0.42
1:A:191:LYS:O	1:A:192:LEU:C	2.62	0.42
1:B:37:HIS:CD2	1:B:37:HIS:C	2.96	0.42
1:B:96:LYS:HD2	1:B:98:ARG:HE	1.84	0.42
1:B:118:ILE:HD13	1:B:142:ILE:HD11	1.96	0.42
1:C:176:ILE:HG23	1:C:214:TYR:HB2	2.00	0.42
1:D:26:LEU:HG	1:D:37:HIS:HB2	2.02	0.42
1:D:35:VAL:CG1	1:D:224:LEU:HD21	2.44	0.42
1:D:251:ASN:O	1:D:252:SER:HB3	2.18	0.42
1:F:203:ARG:HH11	1:F:203:ARG:HG3	1.67	0.42
1:A:17:LYS:HE3	1:A:152:TYR:OH	2.19	0.42
1:B:182:ILE:O	1:B:183:SER:C	2.63	0.42
1:B:296:ILE:HG22	1:B:297:LEU:HD12	2.01	0.42
1:D:305:GLU:O	1:D:308:LYS:HE3	2.20	0.42
1:F:244:TYR:HB2	1:F:246:PHE:CE2	2.54	0.42
1:F:261:ASP:CB	1:F:292:LYS:HE2	2.49	0.42
1:A:196:ASP:O	1:A:199:ASN:N	2.52	0.42
1:C:176:ILE:HD11	1:C:281:LEU:HD11	2.02	0.42
1:D:27:VAL:HG13	1:D:35:VAL:CG1	2.50	0.42
1:D:56:ILE:O	1:D:58:PRO:HD3	2.20	0.42
1:A:31:SER:HA	1:A:32:PRO:HD2	1.91	0.42
1:B:123:TYR:CB	1:B:124:GLU:CB	2.97	0.42
1:B:217:VAL:HG21	1:B:223:ILE:CG1	2.49	0.42
1:C:178:THR:O	1:C:179:GLY:C	2.63	0.42
1:C:208:THR:HA	1:C:239:ASN:ND2	2.35	0.42
1:C:304:ASP:HB3	1:C:307:LYS:CE	2.49	0.42
1:D:55:GLY:CA	1:D:154:THR:OG1	2.68	0.42
1:D:123:TYR:O	1:D:124:GLU:CB	2.68	0.42
1:D:205:SER:OG	4:D:337:HOH:O	2.22	0.42
1:F:26:LEU:HD22	1:F:225:TYR:H	1.85	0.42
1:F:293:VAL:O	1:F:293:VAL:HG12	2.20	0.42
1:B:245:VAL:HG21	1:B:259:VAL:HA	2.02	0.42
1:D:60:TYR:HD2	1:D:61:ASN:HA	1.84	0.42
2:D:415:FAD:H9	2:D:415:FAD:H1'1	1.76	0.42
1:E:10:TYR:CE2	1:E:16:LEU:HD13	2.55	0.42
1:A:189:LEU:O	1:A:193:PHE:HD2	2.03	0.41
1:B:94:ILE:C	1:B:95:LYS:HG2	2.45	0.41
1:C:101:ARG:NH2	1:C:137:TYR:HD2	2.18	0.41
1:D:258:TYR:O	1:D:261:ASP:HB2	2.20	0.41
1:E:24:ILE:HG22	1:E:25:ASN:N	2.35	0.41
1:D:288:SER:O	1:D:289:ILE:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:THR:O	1:E:181:GLY:C	2.63	0.41
1:F:28:ARG:CB	1:F:29:PRO:HD2	2.47	0.41
1:B:31:SER:HA	1:B:32:PRO:HD2	1.67	0.41
1:B:165:ASP:CB	1:E:203:ARG:NH2	2.82	0.41
1:E:180:THR:C	1:E:182:ILE:N	2.76	0.41
1:A:184:PRO:O	1:A:187:SER:HB3	2.20	0.41
1:B:195:TYR:CG	1:B:196:ASP:N	2.88	0.41
1:D:101:ARG:CG	2:D:415:FAD:H4'	2.44	0.41
1:E:122:LYS:CD	1:E:135:TYR:CE2	3.02	0.41
1:B:202:ASN:C	1:B:204:ASN:CG	2.88	0.41
1:C:57:ILE:HA	1:C:100:ALA:HB2	2.01	0.41
1:C:166:ALA:C	1:C:167:ILE:CG2	2.88	0.41
1:F:114:LEU:C	1:F:114:LEU:HD12	2.45	0.41
1:A:293:VAL:C	1:A:296:ILE:H	2.28	0.41
1:B:97:GLN:O	1:B:97:GLN:CG	2.68	0.41
1:E:123:TYR:CZ	1:E:134:ASN:HB3	2.56	0.41
1:A:10:TYR:CD1	1:A:155:GLY:HA2	2.52	0.41
1:B:118:ILE:HG21	1:B:142:ILE:HD13	2.03	0.41
1:B:203:ARG:HD2	1:B:205:SER:N	2.31	0.41
1:A:293:VAL:CA	1:A:296:ILE:HB	2.51	0.41
1:B:290:ARG:CZ	1:B:313:VAL:HG21	2.51	0.41
1:C:50:GLU:OE1	1:C:191:LYS:HD2	2.21	0.41
1:D:173:PHE:HB2	1:D:211:ILE:HG12	2.02	0.41
1:E:114:LEU:O	1:E:114:LEU:CD1	2.68	0.41
1:A:192:LEU:HD13	1:A:211:ILE:HD11	2.03	0.41
1:B:56:ILE:HG12	1:B:153:LEU:HD22	2.02	0.41
1:B:203:ARG:HD3	1:B:203:ARG:C	2.45	0.41
1:B:277:TYR:O	1:B:278:LYS:C	2.64	0.41
1:C:182:ILE:HB	1:C:215:TYR:CZ	2.56	0.41
1:C:261:ASP:O	1:C:265:LYS:N	2.42	0.41
1:D:108:SER:HB2	1:D:190:LYS:HB3	2.03	0.41
1:E:24:ILE:O	1:E:36:TYR:HD2	2.04	0.41
1:E:39:GLU:OE2	1:E:113:ASN:ND2	2.48	0.41
1:E:193:PHE:O	1:E:195:TYR:N	2.53	0.41
1:E:280:GLU:OE2	1:E:310:ARG:CB	2.69	0.41
1:E:305:GLU:O	1:E:309:LYS:CG	2.69	0.41
1:F:111:MET:CE	1:F:190:LYS:HD3	2.51	0.41
1:F:218:TYR:CE1	1:F:248:TYR:HB2	2.55	0.41
1:A:173:PHE:HB2	1:A:211:ILE:HG12	2.03	0.41
1:A:271:LEU:CD1	1:A:300:HIS:HB2	2.50	0.41
1:B:183:SER:N	1:B:184:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:TYR:N	1:E:237:PRO:HD3	2.36	0.41
1:E:273:LEU:O	1:E:277:TYR:HB2	2.21	0.41
1:F:57:ILE:HA	1:F:58:PRO:HD3	1.70	0.41
1:C:293:VAL:O	1:C:297:LEU:HD13	2.20	0.40
1:D:138:CYS:N	2:D:415:FAD:O1P	2.49	0.40
1:D:203:ARG:HE	1:D:204:ASN:CA	2.34	0.40
1:E:37:HIS:CE1	1:E:115:SER:HB2	2.56	0.40
1:B:202:ASN:C	1:B:204:ASN:OD1	2.64	0.40
1:C:307:LYS:HB2	1:C:307:LYS:HE3	1.51	0.40
1:D:246:PHE:C	1:D:248:TYR:N	2.78	0.40
1:C:200:LEU:CD1	1:C:231:TYR:CZ	3.00	0.40
1:E:11:THR:OG1	1:E:13:LYS:HG2	2.21	0.40
1:E:35:VAL:HG22	1:E:119:LYS:HA	2.02	0.40
1:E:101:ARG:HB2	1:E:103:TYR:CE1	2.56	0.40
1:E:126:THR:HB	1:F:290:ARG:HH22	1.87	0.40
1:A:293:VAL:HA	1:A:296:ILE:HB	2.02	0.40
1:B:30:ASN:HB2	1:B:221:ASP:OD2	2.21	0.40
1:C:199:ASN:OD1	1:C:201:TYR:HE2	1.99	0.40
1:C:204:ASN:O	1:C:204:ASN:CG	2.64	0.40
1:A:6:PHE:CD2	1:A:47:LYS:HB3	2.57	0.40
1:E:26:LEU:CG	1:E:37:HIS:HB2	2.46	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	256/316 (81%)	235 (92%)	20 (8%)	1 (0%)	30	65
1	B	256/316 (81%)	231 (90%)	19 (7%)	6 (2%)	5	25
1	C	255/316 (81%)	238 (93%)	15 (6%)	2 (1%)	16	50
1	D	259/316 (82%)	236 (91%)	20 (8%)	3 (1%)	10	40

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	251/316 (79%)	230 (92%)	20 (8%)	1 (0%)	30	65
1	F	245/316 (78%)	219 (89%)	23 (9%)	3 (1%)	10	40
All	All	1522/1896 (80%)	1389 (91%)	117 (8%)	16 (1%)	11	43

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	156	ALA
1	B	208	THR
1	C	167	ILE
1	D	58	PRO
1	F	293	VAL
1	B	5	ASN
1	B	97	GLN
1	B	305	GLU
1	E	291	TYR
1	F	155	GLY
1	C	6	PHE
1	D	247	SER
1	D	296	ILE
1	B	155	GLY
1	B	288	SER
1	F	296	ILE

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	244/295 (83%)	221 (91%)	23 (9%)	8	32
1	B	248/295 (84%)	213 (86%)	35 (14%)	3	16
1	C	244/295 (83%)	222 (91%)	22 (9%)	9	34
1	D	250/295 (85%)	232 (93%)	18 (7%)	13	43
1	E	243/295 (82%)	220 (90%)	23 (10%)	8	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	235/295 (80%)	210 (89%)	25 (11%)	6	27
All	All	1464/1770 (83%)	1318 (90%)	146 (10%)	7	29

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	7	ILE
1	A	26	LEU
1	A	61	ASN
1	A	97	GLN
1	A	110	ASN
1	A	116	VAL
1	A	134	ASN
1	A	147	ILE
1	A	165	ASP
1	A	167	ILE
1	A	171	THR
1	A	200	LEU
1	A	208	THR
1	A	220	GLU
1	A	234	LYS
1	A	273	LEU
1	A	278	LYS
1	A	287	LYS
1	A	290	ARG
1	A	294	MET
1	A	296	ILE
1	A	297	LEU
1	B	7	ILE
1	B	21	VAL
1	B	28	ARG
1	B	35	VAL
1	B	37	HIS
1	B	53	THR
1	B	61	ASN
1	B	98	ARG
1	B	99	CYS
1	B	109	ASN
1	B	110	ASN
1	B	116	VAL
1	B	124	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	131	ASN
1	B	132	ILE
1	B	134	ASN
1	B	147	ILE
1	B	164	ASN
1	B	167	ILE
1	B	191	LYS
1	B	192	LEU
1	B	201	TYR
1	B	203	ARG
1	B	207	TYR
1	B	212	THR
1	B	222	SER
1	B	226	LEU
1	B	248	TYR
1	B	255	THR
1	B	269	GLU
1	B	275	ASN
1	B	288	SER
1	B	296	ILE
1	B	297	LEU
1	B	298	LYS
1	C	30	ASN
1	C	42	HIS
1	C	49	LEU
1	C	50	GLU
1	C	57	ILE
1	C	61	ASN
1	C	110	ASN
1	C	116	VAL
1	C	143	LYS
1	C	147	ILE
1	C	151	ILE
1	C	171	THR
1	C	176	ILE
1	C	200	LEU
1	C	201	TYR
1	C	220	GLU
1	C	255	THR
1	C	272	ASN
1	C	290	ARG
1	C	300	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	306	LYS
1	C	312	HIS
1	D	4	ASN
1	D	35	VAL
1	D	58	PRO
1	D	99	CYS
1	D	116	VAL
1	D	182	ILE
1	D	201	TYR
1	D	204	ASN
1	D	212	THR
1	D	217	VAL
1	D	226	LEU
1	D	250	GLN
1	D	255	THR
1	D	260	GLN
1	D	287	LYS
1	D	291	TYR
1	D	292	LYS
1	D	294	MET
1	E	7	ILE
1	E	11	THR
1	E	33	ASN
1	E	43	ASN
1	E	61	ASN
1	E	97	GLN
1	E	104	SER
1	E	114	LEU
1	E	118	ILE
1	E	126	THR
1	E	151	ILE
1	E	164	ASN
1	E	174	ILE
1	E	187	SER
1	E	200	LEU
1	E	203	ARG
1	E	220	GLU
1	E	241	ASN
1	E	242	ILE
1	E	243	HIS
1	E	287	LYS
1	E	295	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	313	VAL
1	F	9	LEU
1	F	11	THR
1	F	28	ARG
1	F	31	SER
1	F	35	VAL
1	F	45	LEU
1	F	101	ARG
1	F	116	VAL
1	F	147	ILE
1	F	153	LEU
1	F	171	THR
1	F	174	ILE
1	F	182	ILE
1	F	199	ASN
1	F	203	ARG
1	F	217	VAL
1	F	222	SER
1	F	223	ILE
1	F	226	LEU
1	F	256	SER
1	F	266	ARG
1	F	288	SER
1	F	292	LYS
1	F	296	ILE
1	F	297	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	GLN
1	A	170	ASN
1	A	204	ASN
1	A	206	ASN
1	A	233	GLN
1	A	239	ASN
1	A	241	ASN
1	A	300	HIS
1	B	30	ASN
1	B	43	ASN
1	B	61	ASN
1	B	110	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	131	ASN
1	B	134	ASN
1	B	148	ASN
1	B	164	ASN
1	B	168	GLN
1	B	170	ASN
1	B	202	ASN
1	B	206	ASN
1	B	239	ASN
1	B	243	HIS
1	B	260	GLN
1	B	272	ASN
1	C	30	ASN
1	C	33	ASN
1	C	121	HIS
1	C	134	ASN
1	C	172	ASN
1	C	202	ASN
1	C	206	ASN
1	C	241	ASN
1	D	5	ASN
1	D	30	ASN
1	D	43	ASN
1	D	125	GLN
1	D	134	ASN
1	D	148	ASN
1	D	170	ASN
1	D	241	ASN
1	D	243	HIS
1	D	260	GLN
1	D	272	ASN
1	E	43	ASN
1	E	52	HIS
1	E	61	ASN
1	E	125	GLN
1	E	144	ASN
1	E	161	ASN
1	E	170	ASN
1	E	172	ASN
1	E	238	ASN
1	E	239	ASN
1	E	243	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	312	HIS
1	F	43	ASN
1	F	97	GLN
1	F	134	ASN
1	F	144	ASN
1	F	148	ASN
1	F	198	ASN
1	F	199	ASN
1	F	202	ASN
1	F	239	ASN
1	F	241	ASN
1	F	272	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	FAD	C	415	-	58,58,58	1.25	5 (8%)	85,89,89	1.54	15 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2P	A	416	-	29,29,29	1.33	5 (17%)	44,45,45	2.05	13 (29%)
2	FAD	E	415	-	58,58,58	1.33	8 (13%)	85,89,89	1.54	17 (20%)
3	A2P	B	416	-	29,29,29	1.37	5 (17%)	44,45,45	1.91	10 (22%)
3	A2P	C	416	-	29,29,29	1.36	5 (17%)	44,45,45	1.93	9 (20%)
2	FAD	A	415	-	58,58,58	1.26	4 (6%)	85,89,89	1.53	15 (17%)
2	FAD	F	415	-	58,58,58	1.41	6 (10%)	85,89,89	1.54	16 (18%)
3	A2P	D	416	-	29,29,29	1.38	5 (17%)	44,45,45	1.89	11 (25%)
2	FAD	B	415	-	58,58,58	1.30	5 (8%)	85,89,89	1.55	18 (21%)
2	FAD	D	415	-	58,58,58	1.26	5 (8%)	85,89,89	1.54	14 (16%)
3	A2P	F	416	-	29,29,29	1.39	4 (13%)	44,45,45	1.86	10 (22%)
3	A2P	E	416	-	29,29,29	1.37	5 (17%)	44,45,45	1.93	10 (22%)

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	FAD	C	415	-	-	13/34/50/50	0/6/6/6
3	A2P	A	416	-	-	8/15/31/31	0/3/3/3
2	FAD	E	415	-	-	16/34/50/50	0/6/6/6
3	A2P	B	416	-	-	3/15/31/31	0/3/3/3
3	A2P	C	416	-	-	6/15/31/31	0/3/3/3
2	FAD	A	415	-	-	16/34/50/50	0/6/6/6
2	FAD	F	415	-	-	13/34/50/50	0/6/6/6
3	A2P	D	416	-	-	5/15/31/31	0/3/3/3
2	FAD	B	415	-	-	13/34/50/50	0/6/6/6
2	FAD	D	415	-	-	9/34/50/50	0/6/6/6
3	A2P	F	416	-	-	7/15/31/31	0/3/3/3
3	A2P	E	416	-	-	6/15/31/31	0/3/3/3

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	415	FAD	C4X-N5	4.89	1.41	1.30
3	F	416	A2P	C5-C4	4.79	1.47	1.39
3	D	416	A2P	C5-C4	4.64	1.47	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	416	A2P	C5-C4	4.61	1.47	1.39
2	A	415	FAD	C4X-N5	4.57	1.40	1.30
3	B	416	A2P	C5-C4	4.56	1.47	1.39
2	F	415	FAD	C4X-N5	4.49	1.40	1.30
3	A	416	A2P	C5-C4	4.43	1.47	1.39
2	C	415	FAD	C4X-N5	4.41	1.40	1.30
3	C	416	A2P	C5-C4	4.39	1.46	1.39
2	E	415	FAD	C4X-N5	4.28	1.40	1.30
2	B	415	FAD	C4X-N5	4.09	1.39	1.30
2	F	415	FAD	P-O3P	4.04	1.63	1.59
2	B	415	FAD	C10-N1	3.89	1.41	1.33
2	C	415	FAD	C10-N1	3.77	1.40	1.33
2	F	415	FAD	C10-N1	3.76	1.40	1.33
2	E	415	FAD	C10-N1	3.73	1.40	1.33
2	F	415	FAD	PA-O3P	3.70	1.63	1.59
2	D	415	FAD	C10-N1	3.51	1.40	1.33
2	A	415	FAD	C10-N1	3.47	1.40	1.33
2	C	415	FAD	C5A-N7A	-3.23	1.33	1.39
2	F	415	FAD	C5A-N7A	-3.18	1.33	1.39
2	E	415	FAD	C5A-N7A	-3.17	1.33	1.39
2	B	415	FAD	C5A-N7A	-3.14	1.33	1.39
2	D	415	FAD	C5A-N7A	-3.07	1.33	1.39
2	A	415	FAD	C5A-N7A	-3.01	1.33	1.39
2	E	415	FAD	P-O3P	2.97	1.62	1.59
3	F	416	A2P	C5-C6	2.83	1.48	1.41
3	B	416	A2P	C5-C6	2.80	1.48	1.41
2	B	415	FAD	P-O3P	2.80	1.62	1.59
3	E	416	A2P	C5-C6	2.70	1.48	1.41
3	A	416	A2P	C5-C6	2.69	1.48	1.41
2	E	415	FAD	PA-O3P	2.68	1.62	1.59
3	D	416	A2P	C5-C6	2.66	1.48	1.41
3	B	416	A2P	C8-N7	2.51	1.36	1.31
3	C	416	A2P	C5-C6	2.48	1.47	1.41
3	C	416	A2P	C5-N7	-2.47	1.34	1.39
3	D	416	A2P	C8-N7	2.46	1.36	1.31
3	E	416	A2P	C8-N7	2.45	1.36	1.31
3	F	416	A2P	C8-N7	2.41	1.36	1.31
3	A	416	A2P	C8-N7	2.39	1.36	1.31
3	C	416	A2P	C8-N7	2.34	1.36	1.31
2	A	415	FAD	C4A-N9A	-2.23	1.33	1.37
3	C	416	A2P	C4-N9	-2.22	1.33	1.37
3	D	416	A2P	C5-N7	-2.21	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	415	FAD	C8A-N9A	-2.21	1.33	1.37
2	D	415	FAD	C4A-N9A	-2.18	1.33	1.37
3	F	416	A2P	C5-N7	-2.18	1.35	1.39
2	C	415	FAD	C4A-N9A	-2.17	1.33	1.37
2	B	415	FAD	C8A-N9A	-2.16	1.33	1.37
3	E	416	A2P	C5-N7	-2.15	1.35	1.39
2	C	415	FAD	C8A-N9A	-2.12	1.33	1.37
3	A	416	A2P	C5-N7	-2.11	1.35	1.39
2	E	415	FAD	O4B-C1B	2.10	1.46	1.42
3	D	416	A2P	C4-N9	-2.10	1.33	1.37
3	A	416	A2P	C4-N9	-2.09	1.33	1.37
2	E	415	FAD	C8A-N9A	-2.08	1.34	1.37
2	D	415	FAD	C8A-N9A	-2.07	1.34	1.37
3	E	416	A2P	C4-N9	-2.05	1.33	1.37
2	E	415	FAD	C4A-N9A	-2.04	1.33	1.37
3	B	416	A2P	C4-N9	-2.02	1.33	1.37
3	B	416	A2P	C5-N7	-2.00	1.35	1.39

All (158) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	416	A2P	C5-C4-N3	-5.91	118.58	126.72
2	F	415	FAD	C5A-C4A-N3A	-5.66	118.93	126.72
3	D	416	A2P	C5-C4-N3	-5.57	119.05	126.72
2	B	415	FAD	C5A-C4A-N3A	-5.51	119.12	126.72
3	B	416	A2P	C5-C4-N3	-5.51	119.13	126.72
3	A	416	A2P	C5-C4-N3	-5.46	119.20	126.72
3	C	416	A2P	C5-C4-N3	-5.39	119.29	126.72
3	E	416	A2P	C5-C4-N3	-5.39	119.30	126.72
2	E	415	FAD	C5A-C4A-N3A	-5.31	119.40	126.72
2	D	415	FAD	C5A-C4A-N3A	-5.30	119.42	126.72
2	C	415	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
2	A	415	FAD	C5A-C4A-N3A	-4.97	119.88	126.72
3	A	416	A2P	O4'-C1'-N9	4.81	117.33	108.09
2	C	415	FAD	N3A-C2A-N1A	-4.81	121.31	128.58
2	A	415	FAD	N3A-C2A-N1A	-4.78	121.34	128.58
3	F	416	A2P	N3-C4-N9	4.69	135.14	127.17
2	E	415	FAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	D	415	FAD	N3A-C2A-N1A	-4.55	121.69	128.58
3	A	416	A2P	N3-C4-N9	4.40	134.65	127.17
3	D	416	A2P	N3-C4-N9	4.37	134.61	127.17
3	C	416	A2P	N3-C4-N9	4.37	134.60	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	416	A2P	O4'-C1'-N9	4.36	116.47	108.09
2	F	415	FAD	N3A-C2A-N1A	-4.36	121.98	128.58
2	B	415	FAD	N3A-C2A-N1A	-4.34	122.01	128.58
3	E	416	A2P	N3-C4-N9	4.28	134.45	127.17
3	B	416	A2P	N3-C4-N9	4.24	134.37	127.17
2	F	415	FAD	N3A-C4A-N9A	3.91	133.82	127.17
3	D	416	A2P	O4'-C1'-N9	3.88	115.54	108.09
2	C	415	FAD	N3A-C4A-N9A	3.77	133.58	127.17
3	E	416	A2P	O4'-C1'-N9	3.75	115.29	108.09
3	B	416	A2P	C2-N3-C4	3.74	120.97	111.83
3	F	416	A2P	C2-N3-C4	3.72	120.93	111.83
2	B	415	FAD	N3A-C4A-N9A	3.71	133.47	127.17
3	B	416	A2P	C4-C5-N7	-3.68	106.38	110.58
3	A	416	A2P	C2-N3-C4	3.68	120.81	111.83
3	D	416	A2P	C2-N3-C4	3.59	120.60	111.83
2	A	415	FAD	C2A-N3A-C4A	3.59	120.59	111.83
2	D	415	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	C	415	FAD	C2A-N3A-C4A	3.57	120.55	111.83
3	F	416	A2P	C4-C5-N7	-3.57	106.50	110.58
2	E	415	FAD	C2A-N3A-C4A	3.57	120.54	111.83
2	F	415	FAD	C2A-N3A-C4A	3.57	120.54	111.83
3	E	416	A2P	C2-N3-C4	3.56	120.53	111.83
2	E	415	FAD	N3A-C4A-N9A	3.54	133.19	127.17
2	B	415	FAD	C2A-N3A-C4A	3.54	120.47	111.83
3	A	416	A2P	C4-C5-N7	-3.51	106.57	110.58
3	E	416	A2P	C4-C5-N7	-3.51	106.57	110.58
2	B	415	FAD	C4-N3-C2	-3.46	119.50	125.64
3	C	416	A2P	C2-N3-C4	3.44	120.22	111.83
3	A	416	A2P	N3-C2-N1	-3.42	123.40	128.58
3	B	416	A2P	N3-C2-N1	-3.41	123.43	128.58
2	D	415	FAD	N3A-C4A-N9A	3.40	132.95	127.17
3	A	416	A2P	C4-N9-C8	3.37	109.28	105.74
3	D	416	A2P	C4-C5-N7	-3.35	106.75	110.58
2	E	415	FAD	C4-N3-C2	-3.33	119.73	125.64
2	A	415	FAD	C4-N3-C2	-3.31	119.76	125.64
3	C	416	A2P	C4-C5-N7	-3.30	106.80	110.58
2	A	415	FAD	N9A-C8A-N7A	-3.30	109.25	113.94
3	E	416	A2P	N3-C2-N1	-3.28	123.61	128.58
2	B	415	FAD	N9A-C8A-N7A	-3.27	109.29	113.94
2	C	415	FAD	N9A-C8A-N7A	-3.27	109.30	113.94
2	D	415	FAD	N9A-C8A-N7A	-3.24	109.33	113.94
2	D	415	FAD	C4-N3-C2	-3.23	119.91	125.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	415	FAD	C4-N3-C2	-3.22	119.93	125.64
3	B	416	A2P	O4'-C1'-N9	3.20	114.23	108.09
2	E	415	FAD	N9A-C8A-N7A	-3.20	109.40	113.94
3	F	416	A2P	N3-C2-N1	-3.18	123.77	128.58
3	C	416	A2P	C4-N9-C8	3.15	109.05	105.74
2	A	415	FAD	N3A-C4A-N9A	3.14	132.51	127.17
3	D	416	A2P	N3-C2-N1	-3.13	123.84	128.58
2	C	415	FAD	C4-N3-C2	-3.11	120.12	125.64
3	E	416	A2P	C4-N9-C8	3.09	108.99	105.74
3	C	416	A2P	N3-C2-N1	-3.09	123.90	128.58
2	F	415	FAD	N9A-C8A-N7A	-3.09	109.55	113.94
3	B	416	A2P	C4-N9-C8	3.01	108.90	105.74
2	B	415	FAD	C5A-N7A-C8A	2.91	108.03	103.45
2	F	415	FAD	C5A-N7A-C8A	2.86	107.95	103.45
2	D	415	FAD	C4X-C4-N3	2.81	120.41	113.25
2	E	415	FAD	C5A-N7A-C8A	2.81	107.86	103.45
3	D	416	A2P	C4-N9-C8	2.79	108.66	105.74
2	D	415	FAD	C4A-C5A-N7A	-2.78	107.40	110.58
2	B	415	FAD	C4A-C5A-N7A	-2.77	107.41	110.58
2	A	415	FAD	C5A-N7A-C8A	2.77	107.80	103.45
2	E	415	FAD	C4X-C4-N3	2.77	120.30	113.25
2	A	415	FAD	C4A-C5A-N7A	-2.77	107.42	110.58
2	B	415	FAD	O4-C4-C4X	-2.76	119.25	126.53
2	D	415	FAD	C5A-N7A-C8A	2.76	107.78	103.45
3	F	416	A2P	C4-N9-C8	2.74	108.62	105.74
2	A	415	FAD	C4X-C10-N10	2.73	120.39	116.48
2	C	415	FAD	C4X-C4-N3	2.71	120.16	113.25
2	E	415	FAD	O4-C4-C4X	-2.71	119.39	126.53
2	A	415	FAD	C4X-C4-N3	2.71	120.14	113.25
3	A	416	A2P	C5-N7-C8	2.70	107.70	103.45
2	F	415	FAD	C4A-C5A-N7A	-2.70	107.49	110.58
3	F	416	A2P	C5-N7-C8	2.69	107.68	103.45
2	E	415	FAD	C4A-C5A-N7A	-2.68	107.52	110.58
3	B	416	A2P	C5-N7-C8	2.68	107.66	103.45
2	C	415	FAD	O4-C4-C4X	-2.65	119.53	126.53
2	F	415	FAD	C4X-C4-N3	2.64	119.97	113.25
2	B	415	FAD	C4X-C4-N3	2.64	119.97	113.25
2	C	415	FAD	C5A-N7A-C8A	2.61	107.55	103.45
3	E	416	A2P	C5-N7-C8	2.59	107.52	103.45
2	D	415	FAD	C10-C4X-N5	-2.58	119.54	124.81
2	C	415	FAD	C5'-C4'-C3'	-2.57	107.38	112.22
3	A	416	A2P	N9-C8-N7	-2.56	110.30	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	415	FAD	O4-C4-C4X	-2.56	119.78	126.53
3	C	416	A2P	C5-N7-C8	2.55	107.45	103.45
2	D	415	FAD	C4X-C10-N10	2.54	120.11	116.48
2	B	415	FAD	C4-C4X-C10	2.51	121.24	116.93
3	B	416	A2P	C6-C5-N7	2.49	136.89	132.09
2	A	415	FAD	C10-C4X-N5	-2.49	119.73	124.81
2	A	415	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	F	415	FAD	C10-C4X-N5	-2.47	119.77	124.81
2	B	415	FAD	C5X-C9A-N10	2.47	120.20	117.97
2	D	415	FAD	C9A-C5X-N5	-2.46	119.84	122.45
2	F	415	FAD	C4X-C10-N10	2.42	119.95	116.48
2	E	415	FAD	C5X-C9A-N10	2.41	120.15	117.97
2	F	415	FAD	O4-C4-C4X	-2.40	120.19	126.53
2	E	415	FAD	O4B-C1B-N9A	2.40	112.70	108.09
3	B	416	A2P	N9-C8-N7	-2.38	110.56	113.94
3	D	416	A2P	C5-N7-C8	2.37	107.17	103.45
3	C	416	A2P	N9-C8-N7	-2.36	110.58	113.94
3	A	416	A2P	C6-C5-N7	2.36	136.64	132.09
2	C	415	FAD	C4A-N9A-C8A	2.36	108.22	105.74
2	F	415	FAD	C9A-C5X-N5	-2.34	119.97	122.45
3	F	416	A2P	O4'-C1'-N9	2.33	112.57	108.09
2	C	415	FAD	C4X-C10-N10	2.31	119.79	116.48
3	E	416	A2P	N9-C8-N7	-2.30	110.67	113.94
2	C	415	FAD	C9A-C5X-N5	-2.28	120.03	122.45
3	E	416	A2P	C6-C5-N7	2.25	136.43	132.09
2	C	415	FAD	C10-C4X-N5	-2.25	120.21	124.81
2	E	415	FAD	C4X-C10-N10	2.25	119.70	116.48
2	C	415	FAD	C4A-C5A-N7A	-2.23	108.03	110.58
2	A	415	FAD	C5X-C9A-N10	2.23	119.98	117.97
3	A	416	A2P	C4'-O4'-C1'	-2.20	104.61	109.47
2	A	415	FAD	C9A-C5X-N5	-2.18	120.14	122.45
2	B	415	FAD	C4X-C10-N10	2.17	119.59	116.48
3	A	416	A2P	O2'-P1-O4P	-2.17	101.59	109.33
2	B	415	FAD	C4X-C10-N1	-2.17	119.27	124.59
2	B	415	FAD	C10-C4X-N5	-2.17	120.38	124.81
2	E	415	FAD	C9A-C5X-N5	-2.16	120.17	122.45
2	F	415	FAD	C4-C4X-C10	2.16	120.63	116.93
3	F	416	A2P	C6-C5-N7	2.14	136.21	132.09
2	F	415	FAD	C5X-C9A-N10	2.13	119.89	117.97
2	E	415	FAD	C4-C4X-C10	2.13	120.58	116.93
3	F	416	A2P	N9-C8-N7	-2.13	110.92	113.94
2	E	415	FAD	C10-C4X-N5	-2.12	120.48	124.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	415	FAD	C9A-C5X-N5	-2.11	120.22	122.45
2	E	415	FAD	C4X-C10-N1	-2.10	119.45	124.59
3	D	416	A2P	C6-C5-N7	2.08	136.09	132.09
2	A	415	FAD	C4A-N9A-C8A	2.06	107.91	105.74
2	F	415	FAD	C4X-C10-N1	-2.05	119.56	124.59
2	B	415	FAD	C3B-C2B-C1B	2.05	105.34	101.46
3	A	416	A2P	C2'-C1'-N9	-2.04	110.40	113.75
3	D	416	A2P	C2'-C1'-N9	-2.03	110.42	113.75
3	D	416	A2P	N9-C8-N7	-2.03	111.06	113.94
2	B	415	FAD	C4A-N9A-C8A	2.02	107.86	105.74
2	D	415	FAD	C4A-N9A-C8A	2.01	107.85	105.74

There are no chirality outliers.

All (115) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	415	FAD	C2'-C1'-N10-C10
2	A	415	FAD	N10-C1'-C2'-O2'
2	A	415	FAD	N10-C1'-C2'-C3'
2	A	415	FAD	C1'-C2'-C3'-O3'
2	A	415	FAD	C1'-C2'-C3'-C4'
2	A	415	FAD	O2'-C2'-C3'-C4'
2	A	415	FAD	C3'-C4'-C5'-O5'
2	A	415	FAD	O4'-C4'-C5'-O5'
2	A	415	FAD	C5'-O5'-P-O3P
2	B	415	FAD	C5B-O5B-PA-O1A
2	B	415	FAD	C5B-O5B-PA-O3P
2	B	415	FAD	C1'-C2'-C3'-O3'
2	B	415	FAD	C1'-C2'-C3'-C4'
2	B	415	FAD	O2'-C2'-C3'-O3'
2	B	415	FAD	O2'-C2'-C3'-C4'
2	C	415	FAD	C5B-O5B-PA-O3P
2	C	415	FAD	N10-C1'-C2'-O2'
2	C	415	FAD	N10-C1'-C2'-C3'
2	C	415	FAD	C1'-C2'-C3'-O3'
2	C	415	FAD	C1'-C2'-C3'-C4'
2	C	415	FAD	O2'-C2'-C3'-O3'
2	C	415	FAD	O2'-C2'-C3'-C4'
2	C	415	FAD	C5'-O5'-P-O3P
2	C	415	FAD	PA-O3P-P-O5'
2	D	415	FAD	C5B-O5B-PA-O2A
2	D	415	FAD	C1'-C2'-C3'-O3'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	415	FAD	C1'-C2'-C3'-C4'
2	D	415	FAD	O2'-C2'-C3'-O3'
2	D	415	FAD	O2'-C2'-C3'-C4'
2	D	415	FAD	C3'-C4'-C5'-O5'
2	E	415	FAD	C5B-O5B-PA-O1A
2	E	415	FAD	C5B-O5B-PA-O2A
2	E	415	FAD	C5B-O5B-PA-O3P
2	E	415	FAD	N10-C1'-C2'-O2'
2	E	415	FAD	N10-C1'-C2'-C3'
2	E	415	FAD	C1'-C2'-C3'-O3'
2	E	415	FAD	C1'-C2'-C3'-C4'
2	E	415	FAD	O2'-C2'-C3'-O3'
2	E	415	FAD	O2'-C2'-C3'-C4'
2	F	415	FAD	O4B-C4B-C5B-O5B
2	F	415	FAD	C1'-C2'-C3'-O3'
2	F	415	FAD	C1'-C2'-C3'-C4'
2	F	415	FAD	O2'-C2'-C3'-O3'
2	F	415	FAD	O2'-C2'-C3'-C4'
2	F	415	FAD	C3'-C4'-C5'-O5'
2	F	415	FAD	O4'-C4'-C5'-O5'
3	A	416	A2P	C5'-O5'-P-OP1
3	A	416	A2P	C5'-O5'-P-OP3
3	A	416	A2P	C5'-O5'-P-OP2
3	A	416	A2P	C2'-C1'-N9-C8
3	C	416	A2P	C2'-C1'-N9-C8
3	D	416	A2P	C2'-C1'-N9-C8
3	F	416	A2P	C5'-O5'-P-OP1
3	F	416	A2P	C5'-O5'-P-OP3
3	F	416	A2P	C2'-C1'-N9-C8
2	A	415	FAD	O2'-C2'-C3'-O3'
2	A	415	FAD	O4B-C4B-C5B-O5B
3	D	416	A2P	O4'-C4'-C5'-O5'
2	A	415	FAD	C3B-C4B-C5B-O5B
3	A	416	A2P	O4'-C4'-C5'-O5'
3	A	416	A2P	C3'-C4'-C5'-O5'
3	D	416	A2P	C3'-C4'-C5'-O5'
3	C	416	A2P	C2'-C1'-N9-C4
3	D	416	A2P	C2'-C1'-N9-C4
3	F	416	A2P	C2'-C1'-N9-C4
2	E	415	FAD	O4'-C4'-C5'-O5'
2	F	415	FAD	C3B-C4B-C5B-O5B
3	B	416	A2P	C2'-C1'-N9-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	416	A2P	C2'-C1'-N9-C8
2	E	415	FAD	C3'-C4'-C5'-O5'
2	B	415	FAD	O4B-C4B-C5B-O5B
3	A	416	A2P	C2'-C1'-N9-C4
2	E	415	FAD	C4'-C5'-O5'-P
2	D	415	FAD	O4'-C4'-C5'-O5'
2	B	415	FAD	C3B-C4B-C5B-O5B
2	A	415	FAD	P-O3P-PA-O5B
2	A	415	FAD	PA-O3P-P-O5'
2	E	415	FAD	P-O3P-PA-O5B
2	E	415	FAD	PA-O3P-P-O5'
3	C	416	A2P	O4'-C4'-C5'-O5'
2	B	415	FAD	N10-C1'-C2'-C3'
3	C	416	A2P	C3'-C4'-C5'-O5'
3	D	416	A2P	C2'-O2'-P1-O4P
3	B	416	A2P	C2'-C1'-N9-C4
3	E	416	A2P	C2'-C1'-N9-C4
2	A	415	FAD	C5B-O5B-PA-O1A
2	A	415	FAD	C5'-O5'-P-O1P
2	B	415	FAD	C5B-O5B-PA-O2A
2	C	415	FAD	C5B-O5B-PA-O1A
2	C	415	FAD	C5'-O5'-P-O1P
2	E	415	FAD	C5'-O5'-P-O1P
2	F	415	FAD	C5B-O5B-PA-O1A
2	F	415	FAD	C5B-O5B-PA-O2A
2	F	415	FAD	C5B-O5B-PA-O3P
2	F	415	FAD	C2'-C1'-N10-C10
2	C	415	FAD	C4'-C5'-O5'-P
3	B	416	A2P	C5'-O5'-P-OP1
2	D	415	FAD	O4B-C4B-C5B-O5B
2	D	415	FAD	C3B-C4B-C5B-O5B
2	C	415	FAD	O4B-C4B-C5B-O5B
3	E	416	A2P	O4'-C4'-C5'-O5'
3	C	416	A2P	C2'-O2'-P1-O4P
3	E	416	A2P	C2'-O2'-P1-O4P
2	B	415	FAD	PA-O3P-P-O1P
3	F	416	A2P	C5'-O5'-P-OP2
2	B	415	FAD	PA-O3P-P-O2P
2	E	415	FAD	PA-O3P-P-O2P
3	E	416	A2P	O4'-C1'-N9-C8
3	F	416	A2P	O4'-C4'-C5'-O5'
3	C	416	A2P	C2'-O2'-P1-O5P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	416	A2P	C2'-O2'-P1-O5P
2	B	415	FAD	N10-C1'-C2'-O2'
2	F	415	FAD	N10-C1'-C2'-O2'
3	F	416	A2P	C3'-C4'-C5'-O5'
3	A	416	A2P	C2'-O2'-P1-O4P

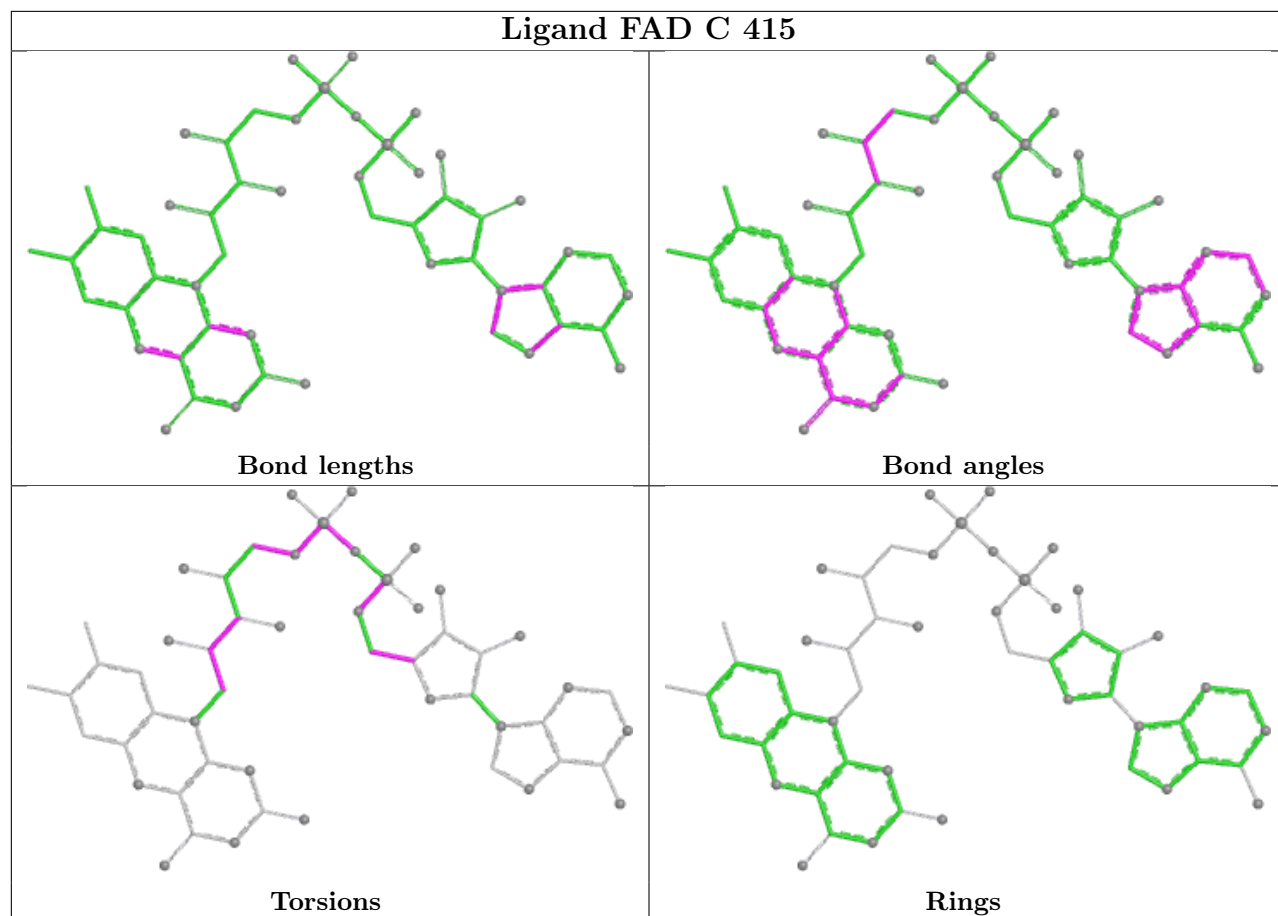
There are no ring outliers.

11 monomers are involved in 38 short contacts:

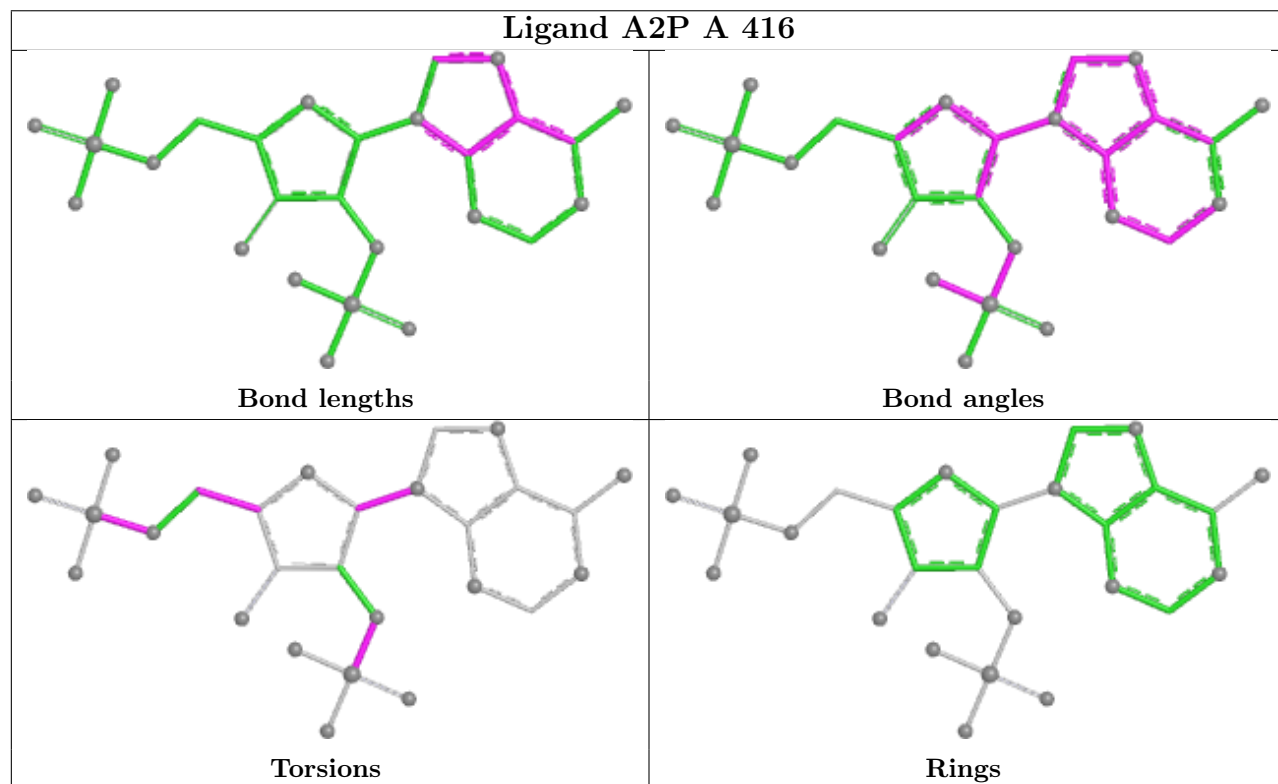
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	415	FAD	2	0
3	A	416	A2P	2	0
2	E	415	FAD	3	0
3	B	416	A2P	3	0
3	C	416	A2P	7	0
2	A	415	FAD	3	0
3	D	416	A2P	5	0
2	B	415	FAD	3	0
2	D	415	FAD	6	0
3	F	416	A2P	2	0
3	E	416	A2P	2	0

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

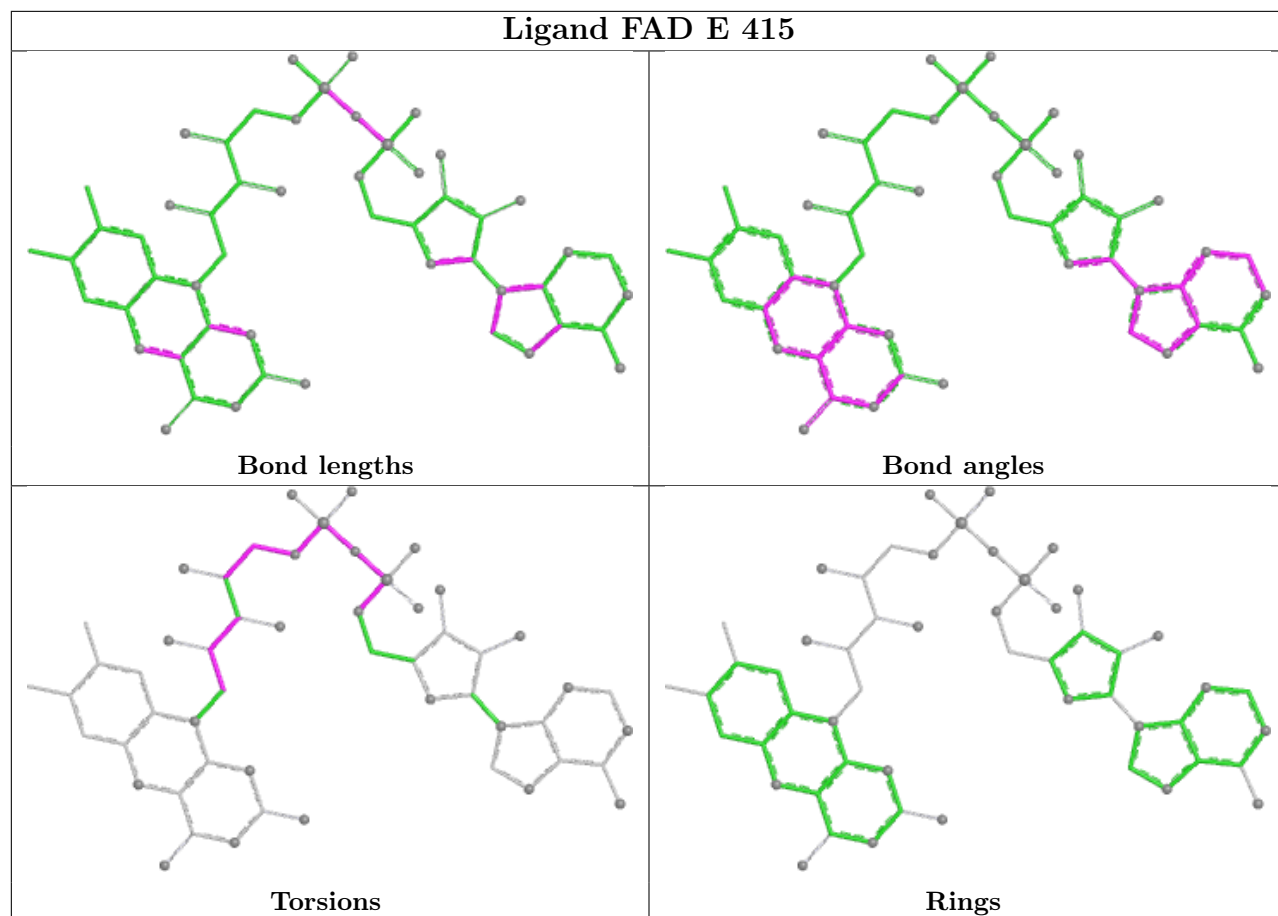
Ligand FAD C 415



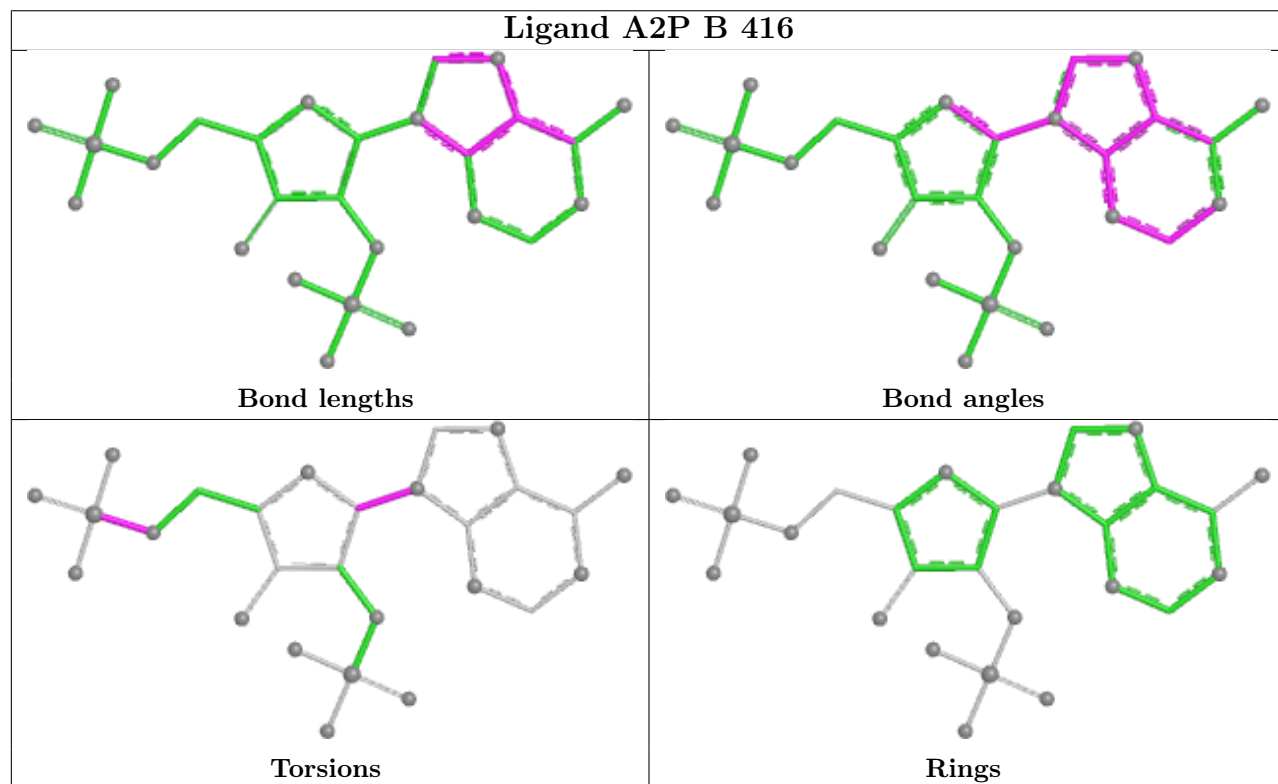
Ligand A2P A 416



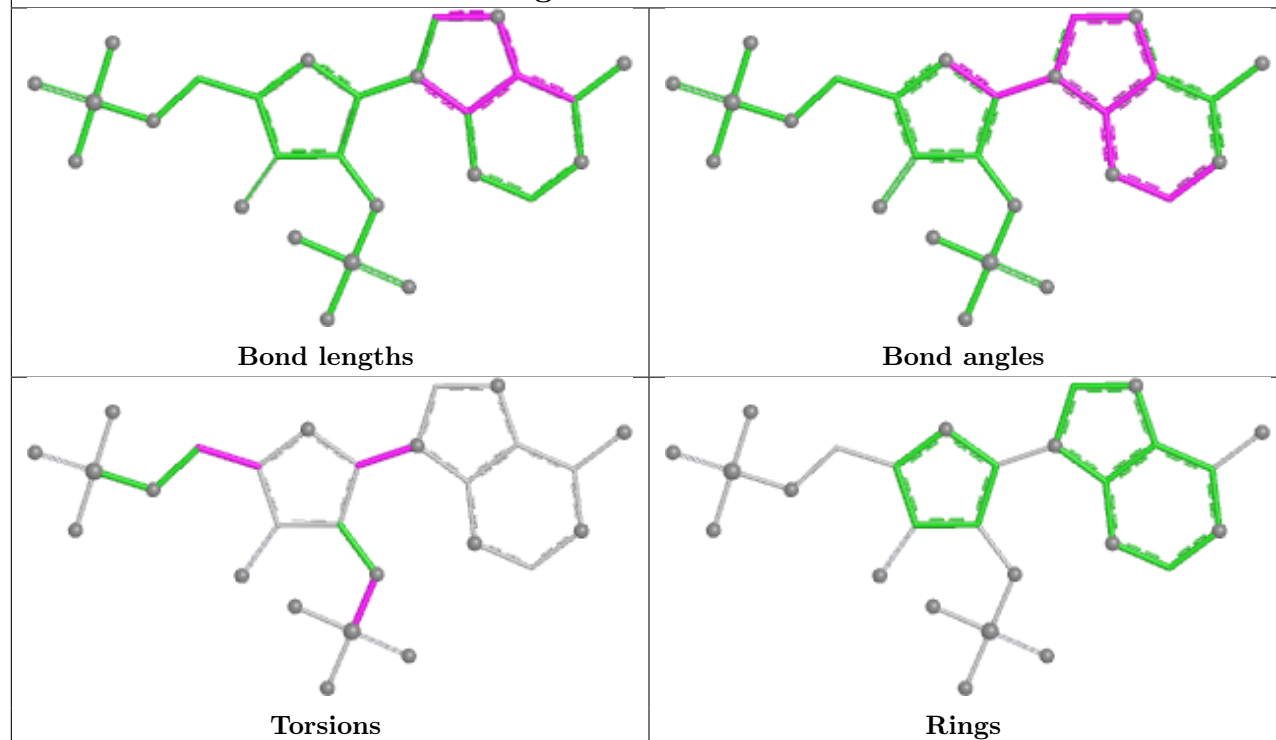
Ligand FAD E 415



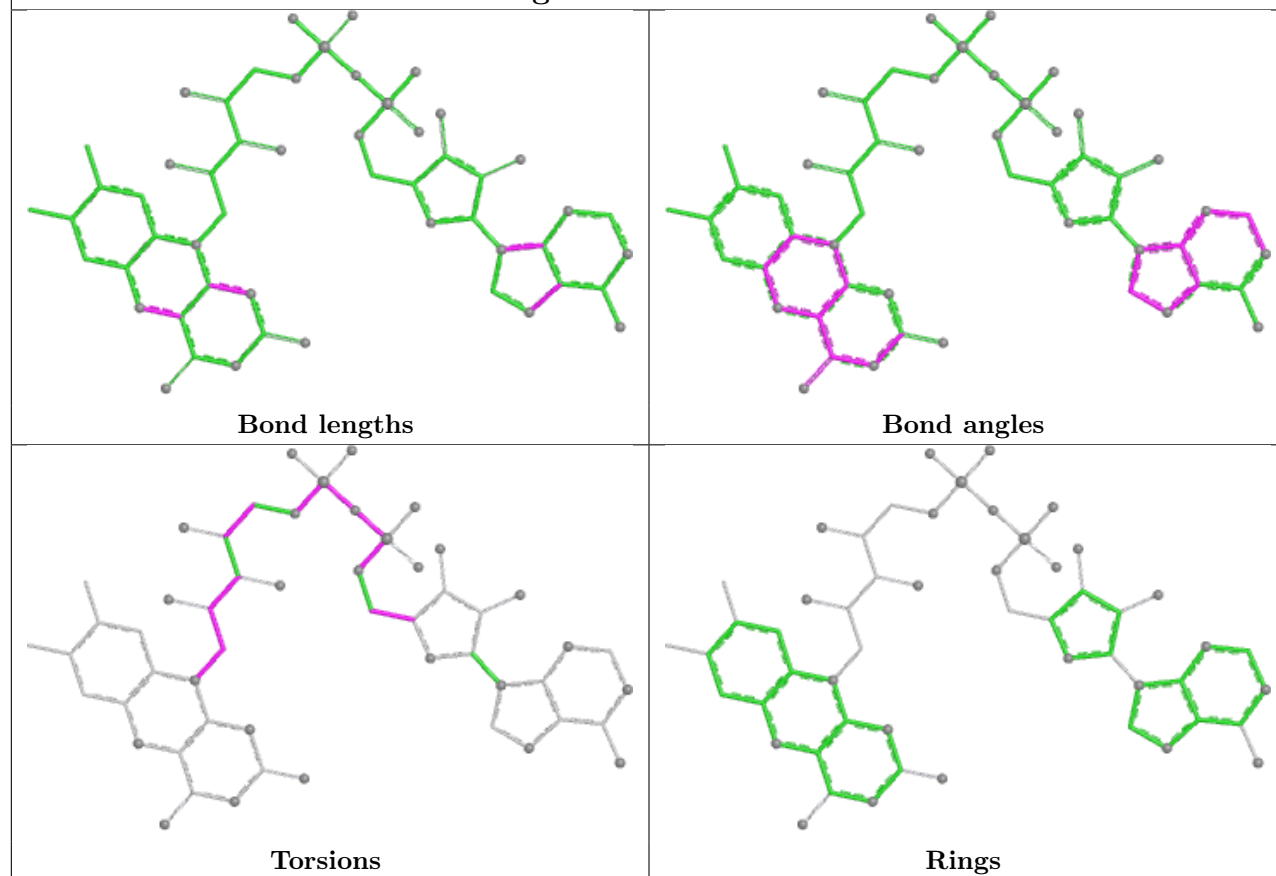
Ligand A2P B 416



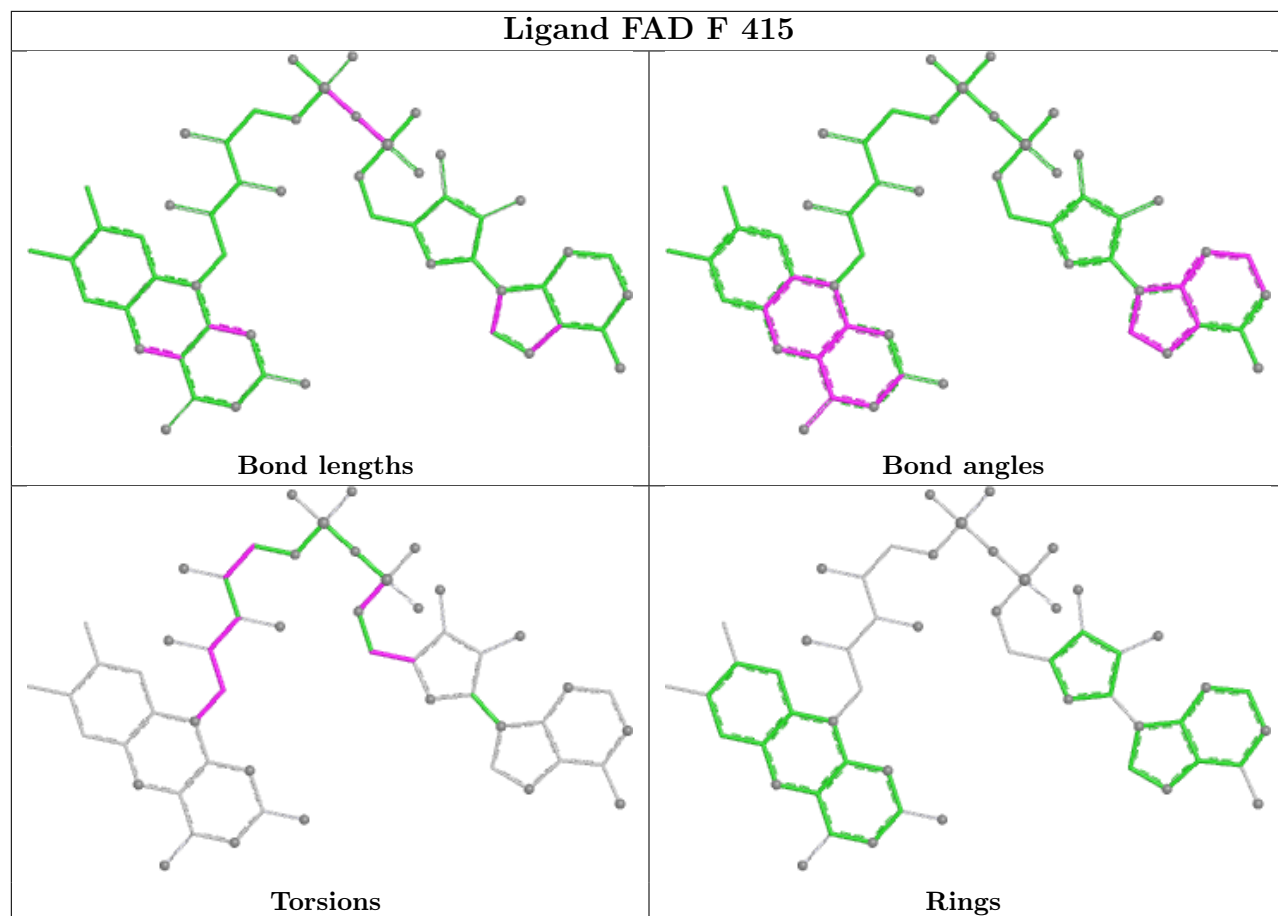
Ligand A2P C 416



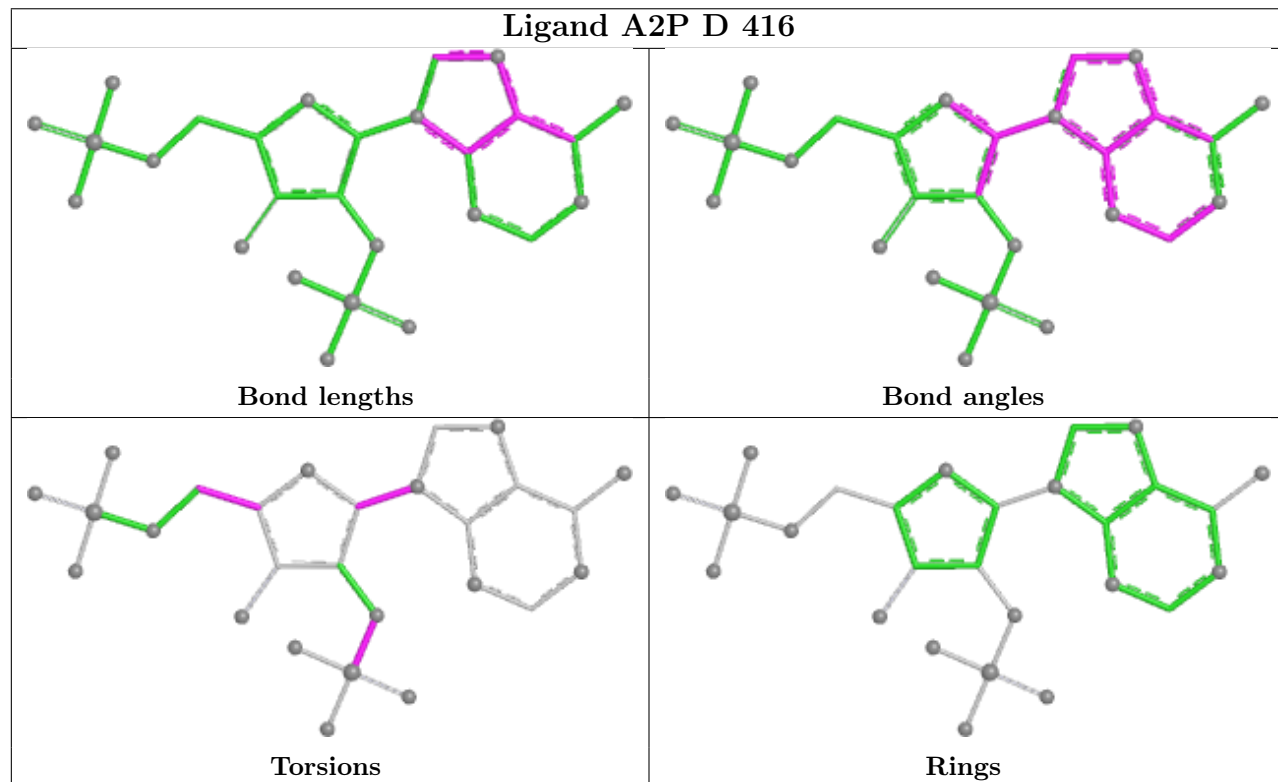
Ligand FAD A 415

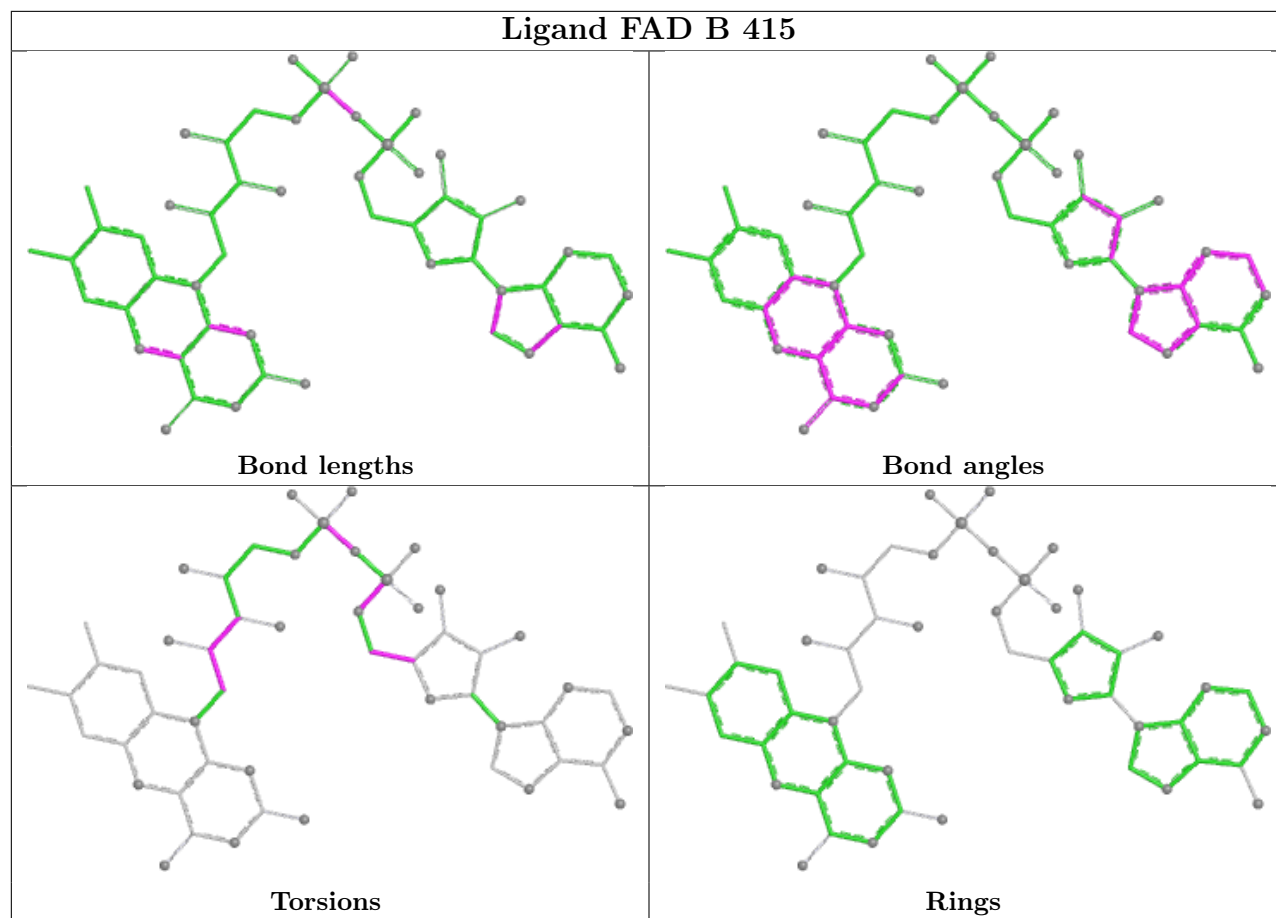


Ligand FAD F 415

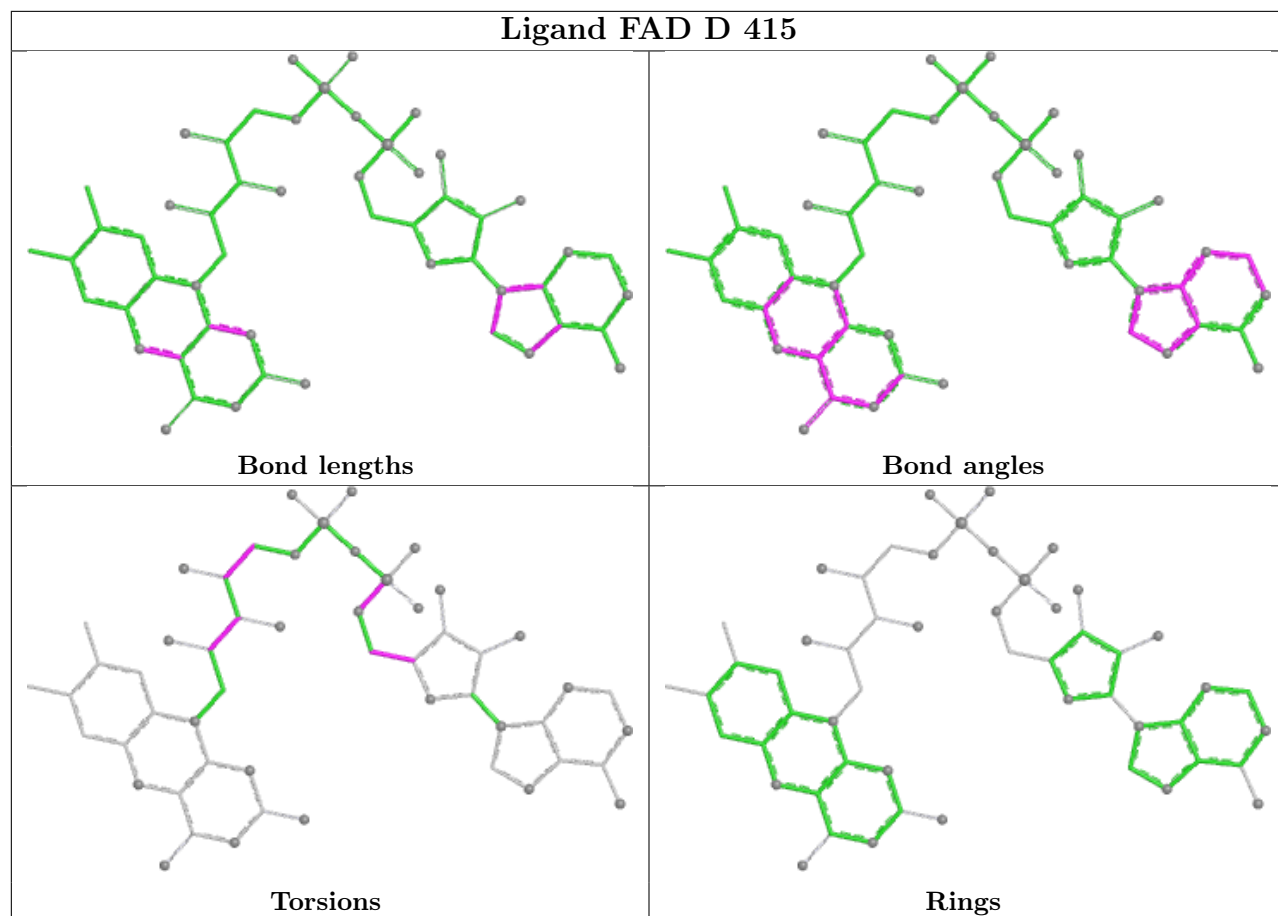


Ligand A2P D 416

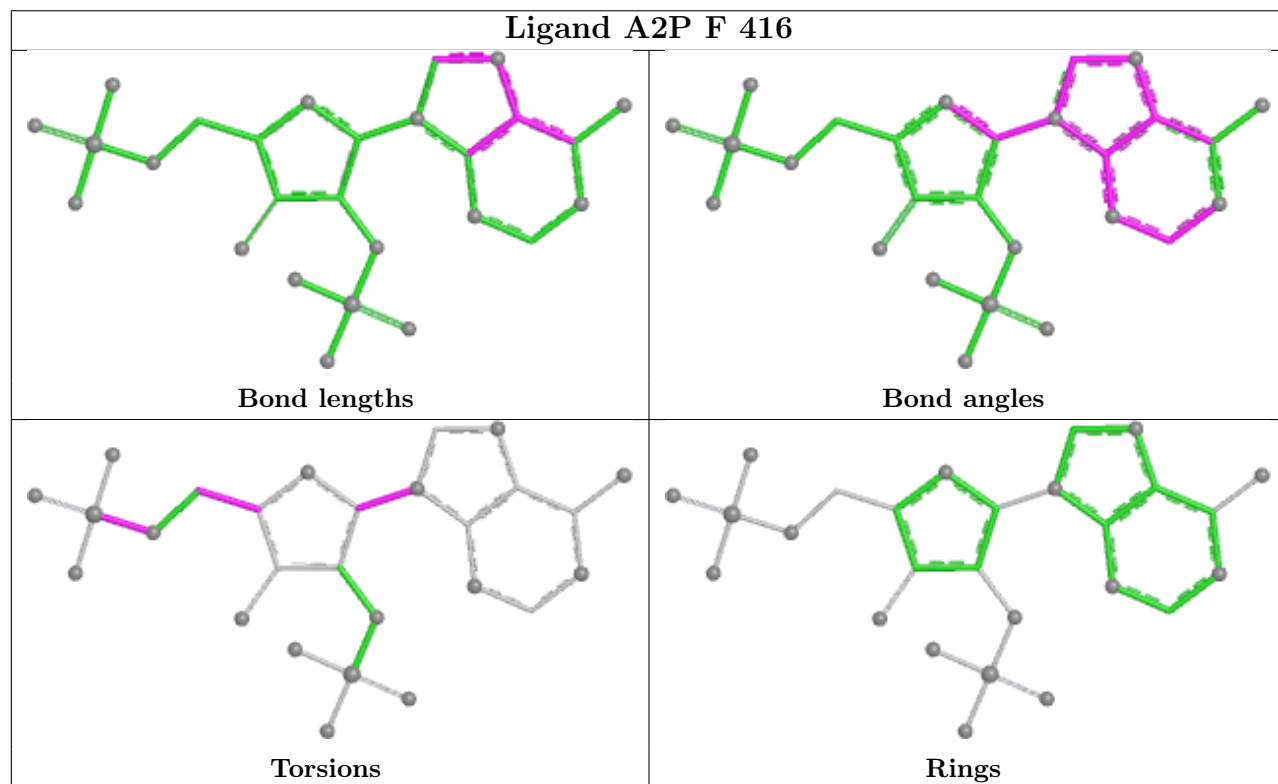


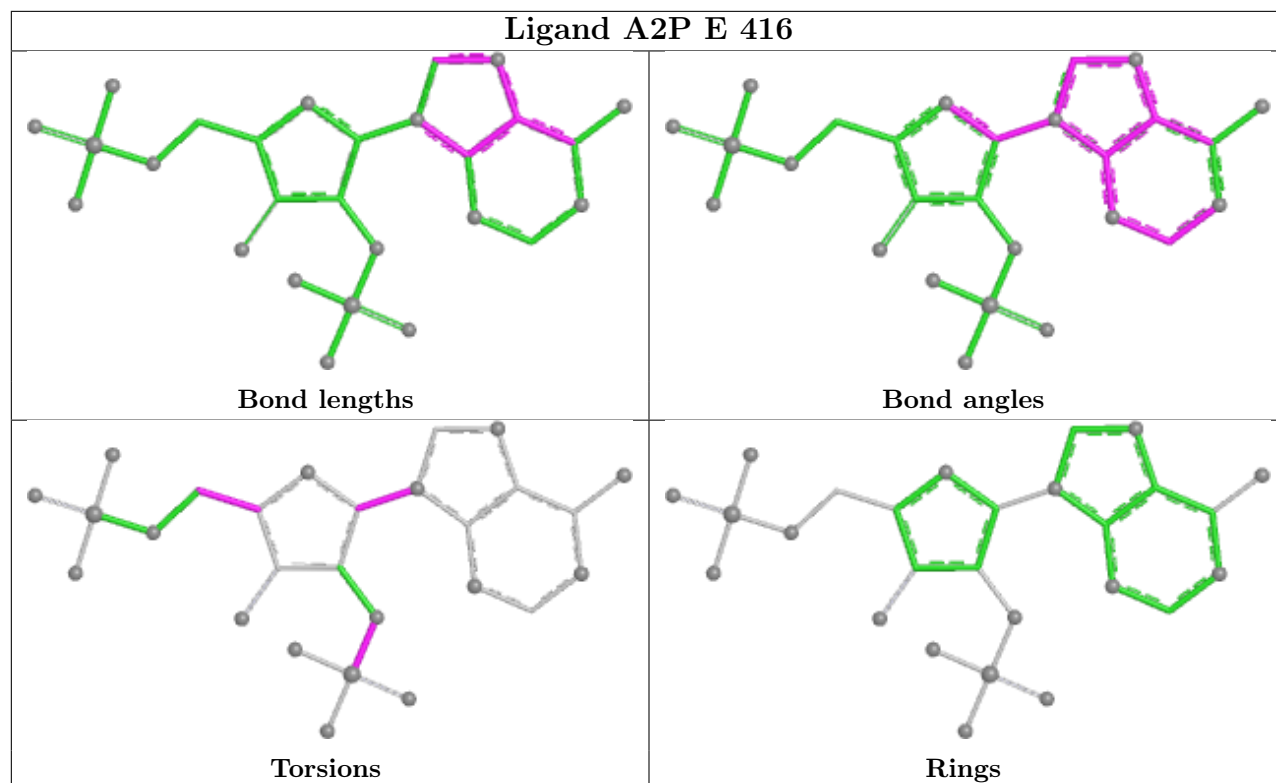


Ligand FAD D 415



Ligand A2P F 416





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	265/316 (83%)	-1.53	0 100 100	22, 42, 74, 89	0
1	B	266/316 (84%)	-1.52	0 100 100	26, 46, 79, 88	0
1	C	265/316 (83%)	-1.61	0 100 100	21, 38, 72, 85	0
1	D	269/316 (85%)	-1.51	0 100 100	23, 44, 78, 87	0
1	E	261/316 (82%)	-1.44	0 100 100	50, 68, 99, 104	0
1	F	257/316 (81%)	-1.42	0 100 100	58, 78, 97, 101	0
All	All	1583/1896 (83%)	-1.51	0 100 100	21, 56, 90, 104	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	FAD	A	415	53/53	0.99	0.03	31,35,39,40	0

Continued on next page...

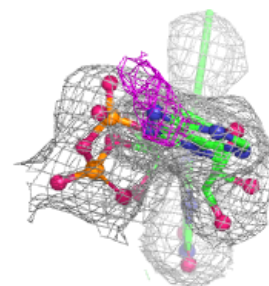
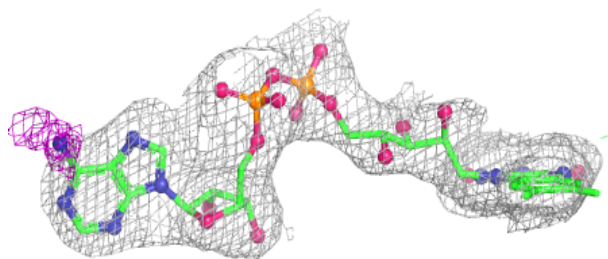
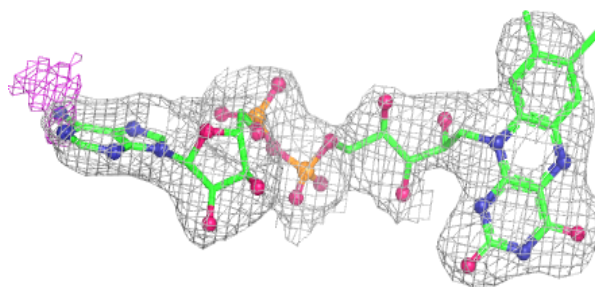
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	E	415	53/53	0.99	0.04	41,58,74,75	0
2	FAD	F	415	53/53	0.99	0.04	66,72,79,81	0
3	A2P	E	416	27/27	0.99	0.03	55,60,67,69	0
3	A2P	F	416	27/27	0.99	0.03	56,69,73,73	0
2	FAD	C	415	53/53	1.00	0.03	15,22,34,35	0
3	A2P	A	416	27/27	1.00	0.02	31,34,41,42	0
3	A2P	B	416	27/27	1.00	0.02	29,38,43,44	0
3	A2P	C	416	27/27	1.00	0.02	20,30,42,44	0
3	A2P	D	416	27/27	1.00	0.03	27,29,35,37	0
2	FAD	D	415	53/53	1.00	0.03	15,30,34,36	0
2	FAD	B	415	53/53	1.00	0.03	23,34,39,40	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.

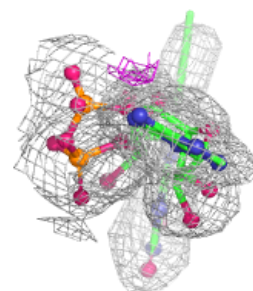
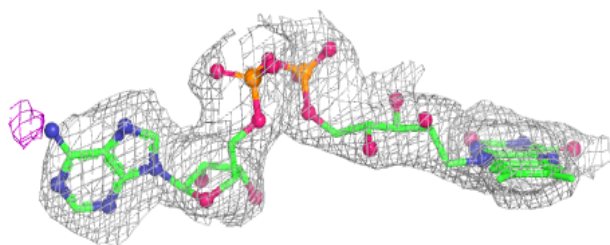
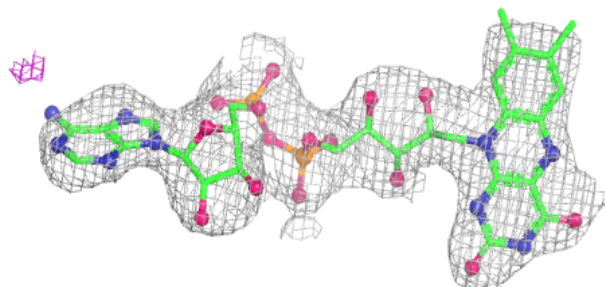
Electron density around FAD A 415:

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

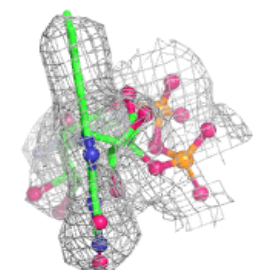
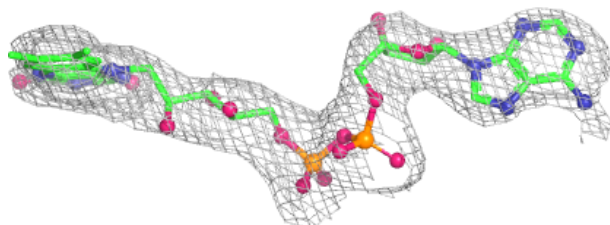
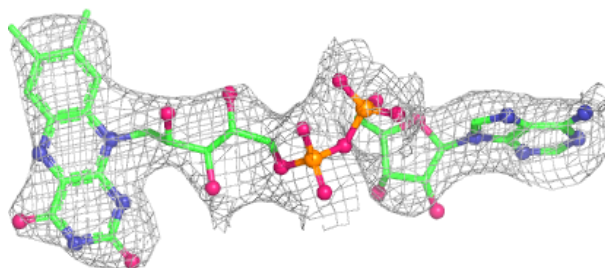


Electron density around FAD E 415:

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

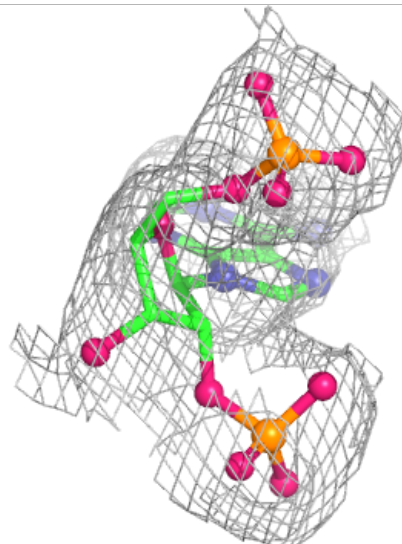
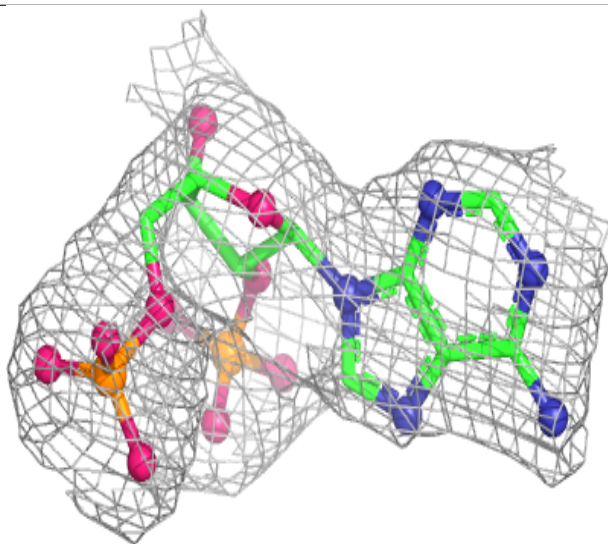
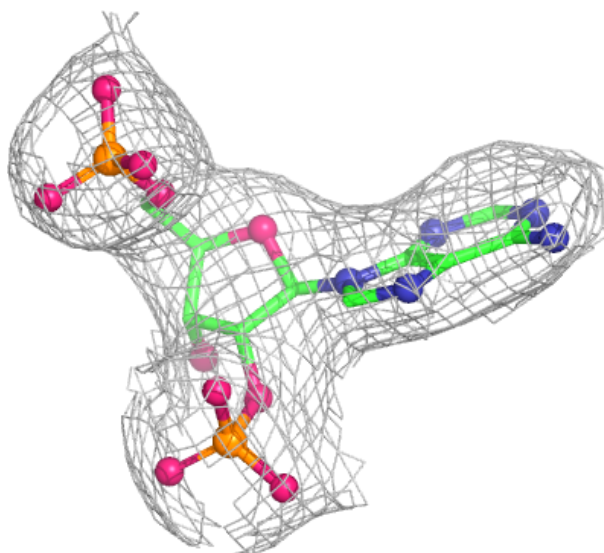
**Electron density around FAD F 415:**

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



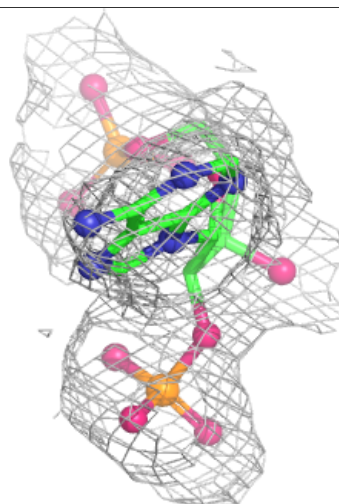
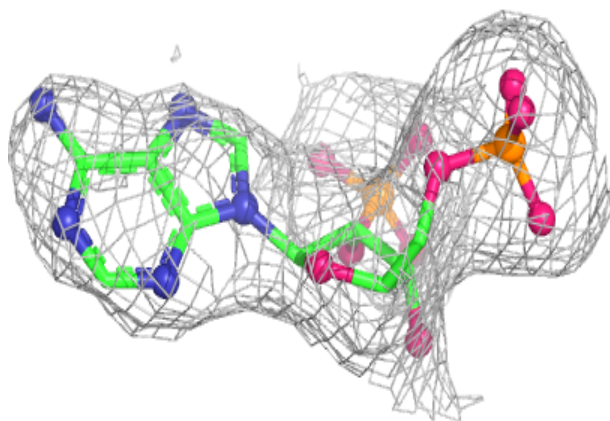
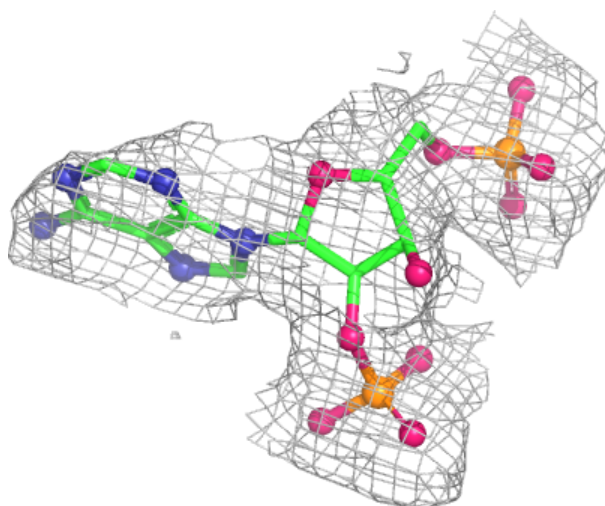
Electron density around A2P E 416:

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



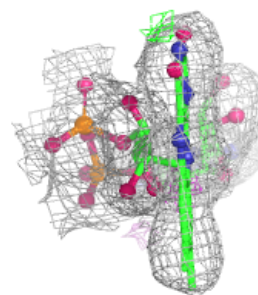
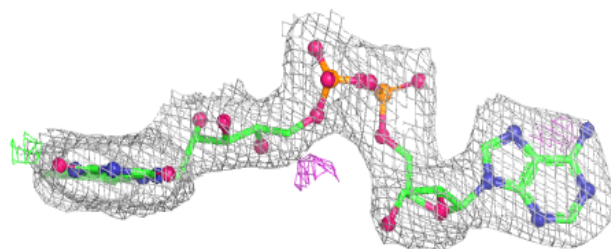
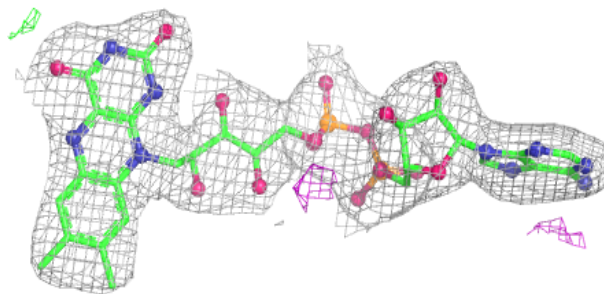
Electron density around A2P F 416:

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



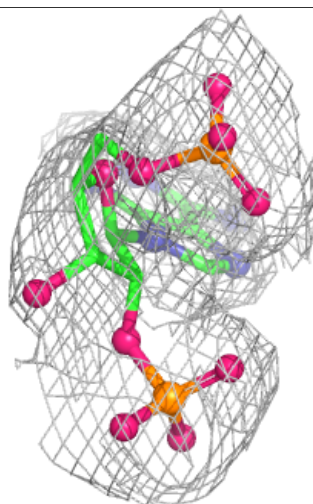
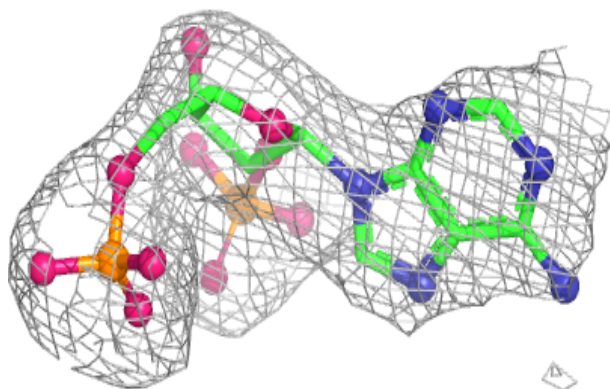
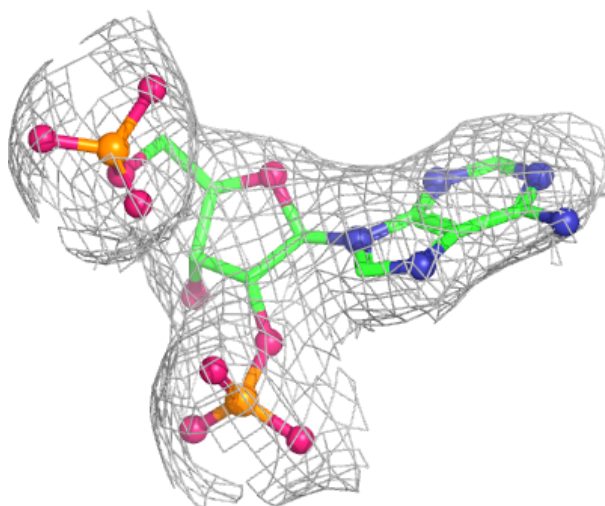
Electron density around FAD C 415:

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



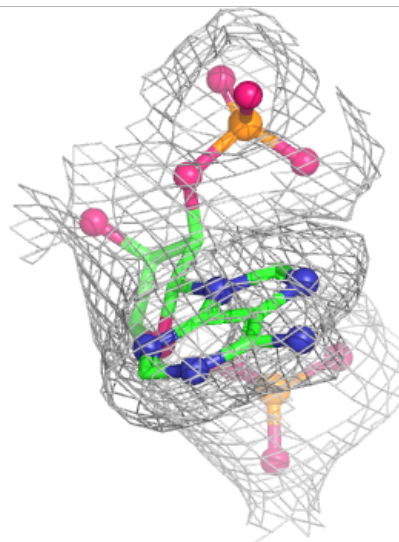
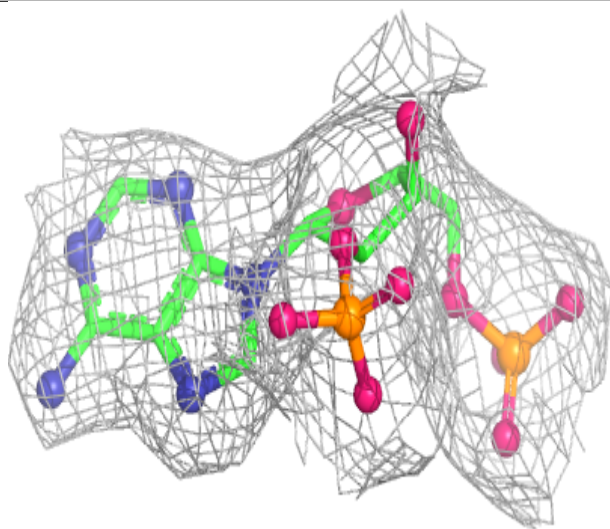
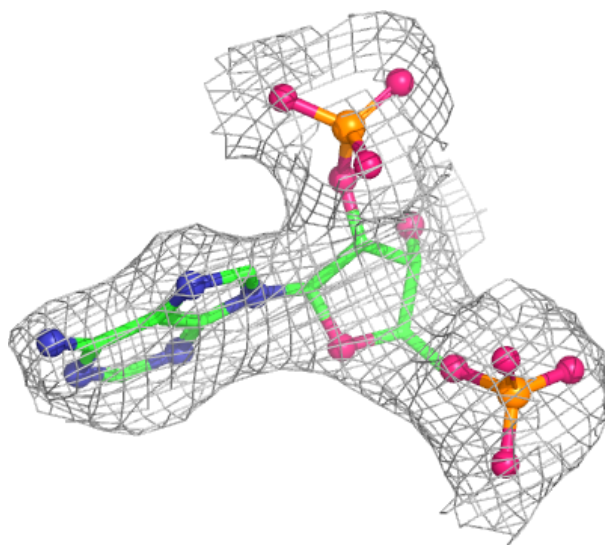
Electron density around A2P A 416:

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



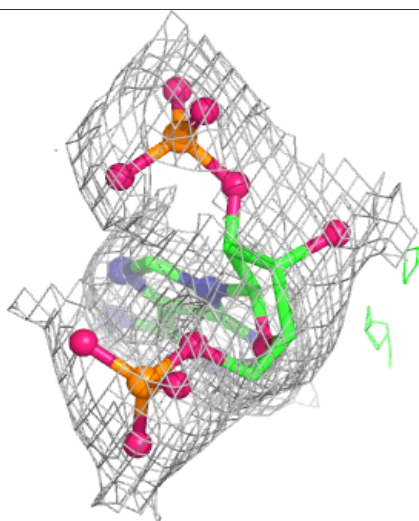
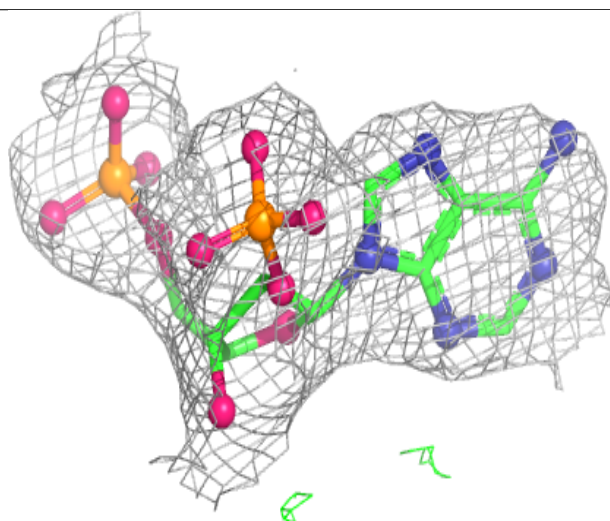
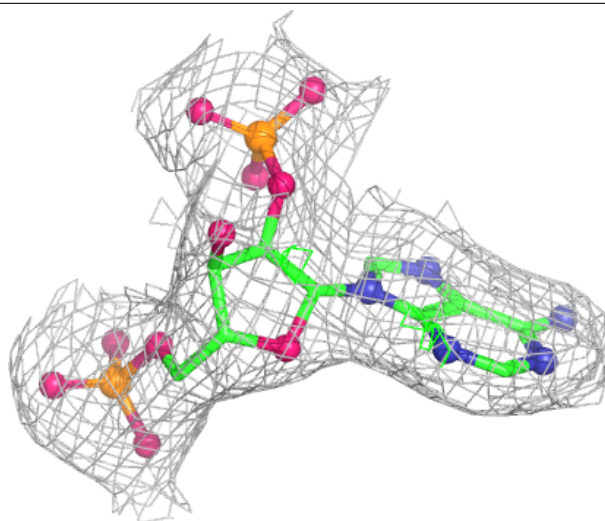
Electron density around A2P B 416:

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



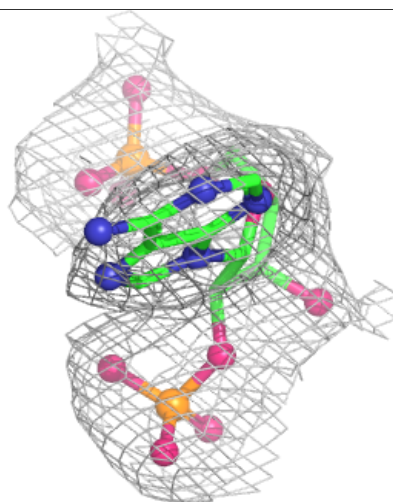
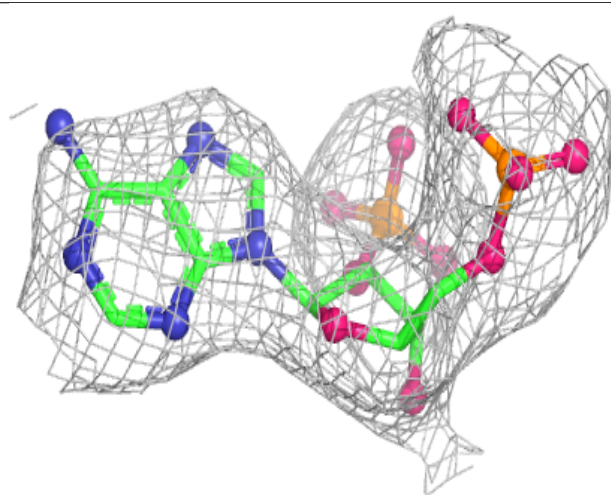
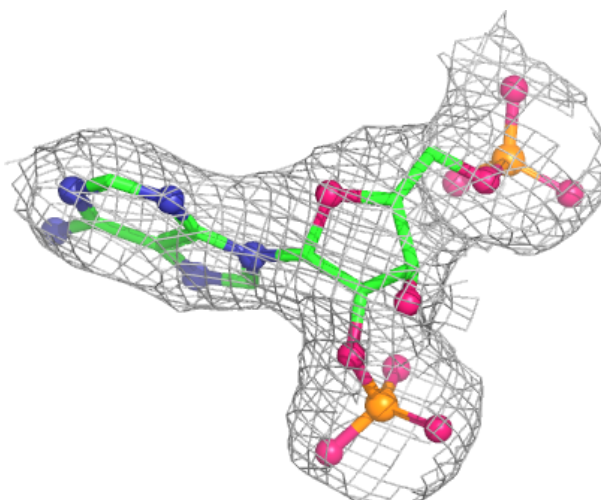
Electron density around A2P C 416:

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



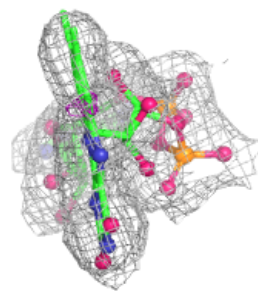
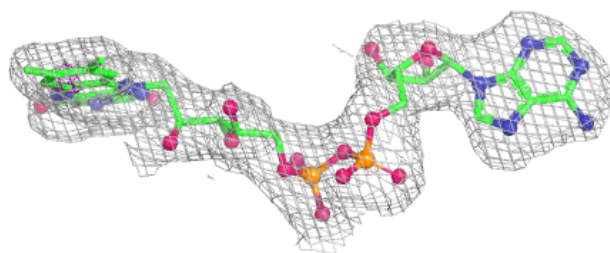
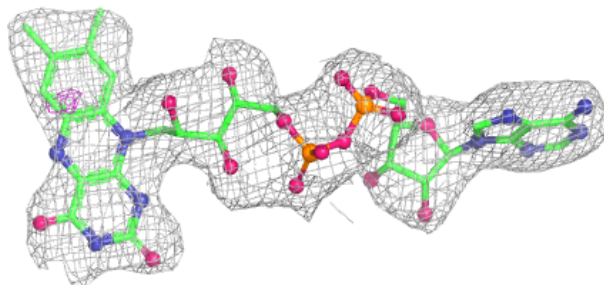
Electron density around A2P D 416:

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

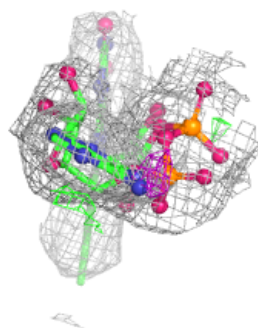
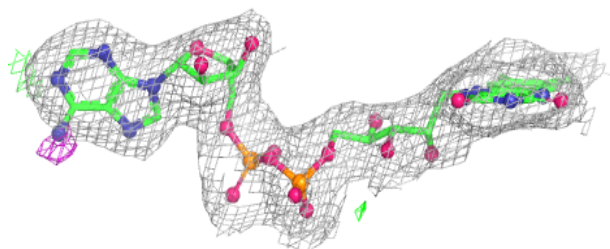
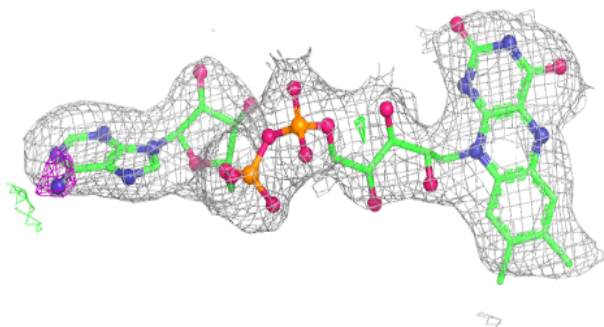


Electron density around FAD D 415:

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

**Electron density around FAD B 415:**

$2mF_o-DF_c$ (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.