Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 02:23 pm BST

PDB ID	:	5NCC
Title	:	Structure of Fatty acid Photodecarboxylase in complex with FAD and palmitic acid
Authors	:	Arnoux, P.; Sorigue, D.; Beisson, F.; Pignol, D.
Deposited on	:	2017-03-03
Resolution	:	3.12 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 following versions of software and data (see references ⓘ) were used in the production of this report:

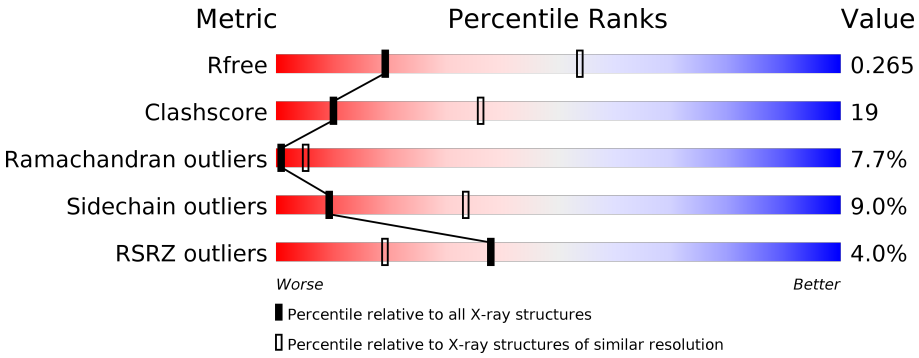
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.12 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}	130704	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)

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 on 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 <=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	594	60% 28% 8%
1	B	594	61% 28% 6%
1	C	594	61% 27% 7%
1	D	594	60% 28% 7%
1	E	594	10% 59% 29% 8%
1	F	594	7% 63% 25% 8%

2 Entry composition (i)

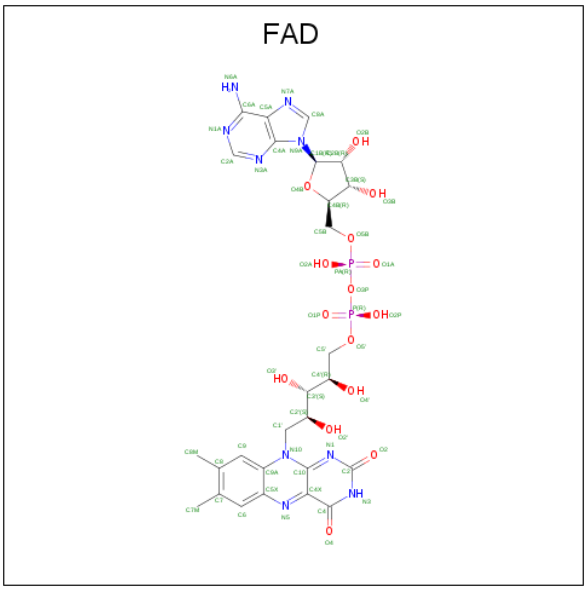
There are 3 unique types of molecules in this entry. The entry contains 26184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty acid Photodecarboxylase.

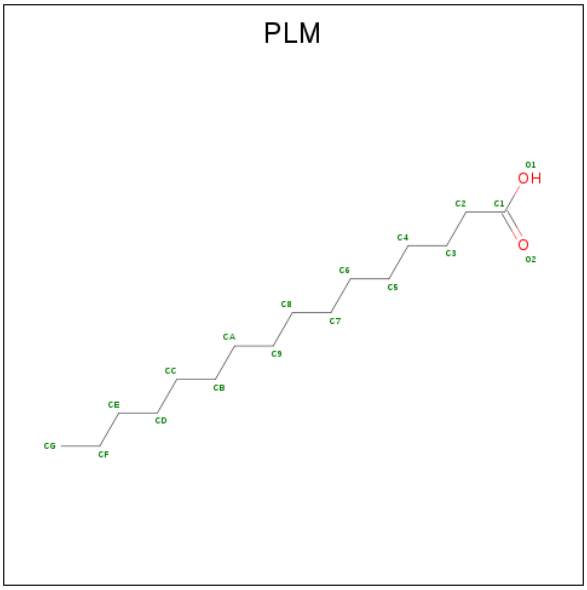
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	B	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	C	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	D	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	E	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	F	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: 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 PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



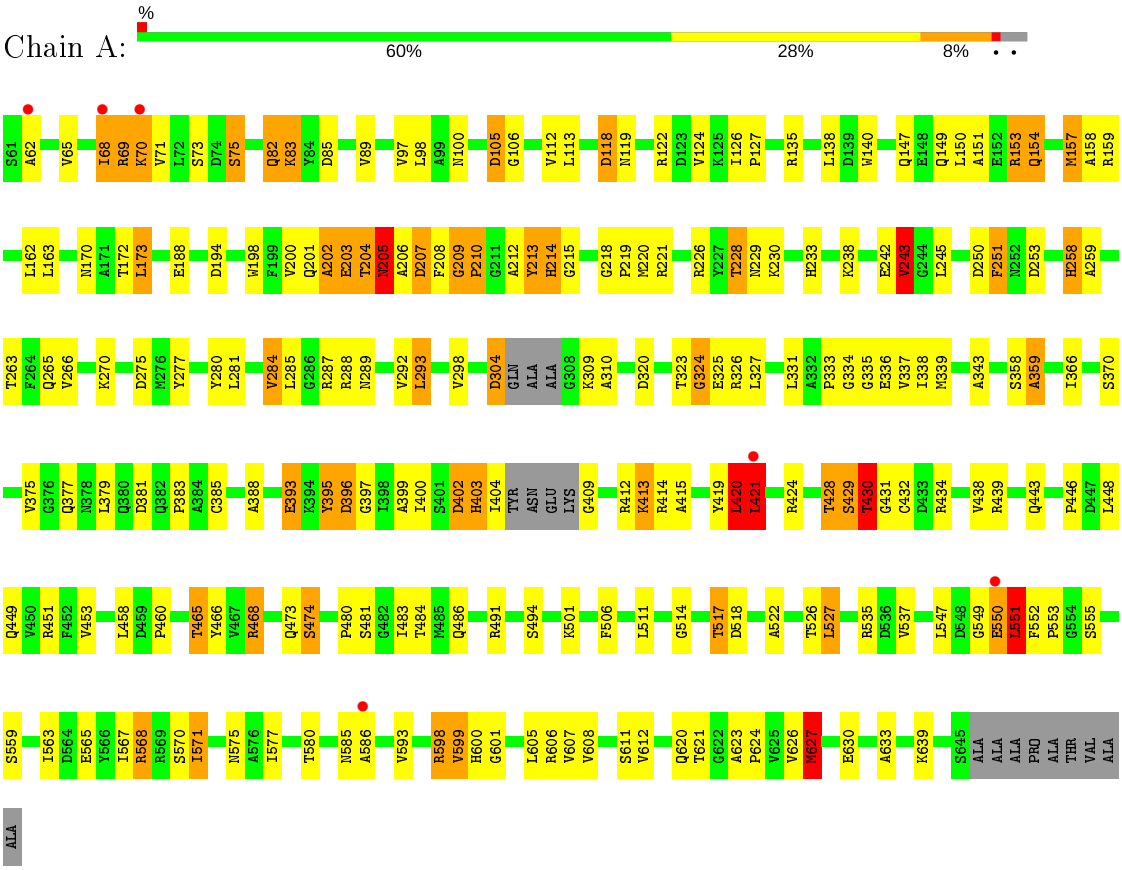
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

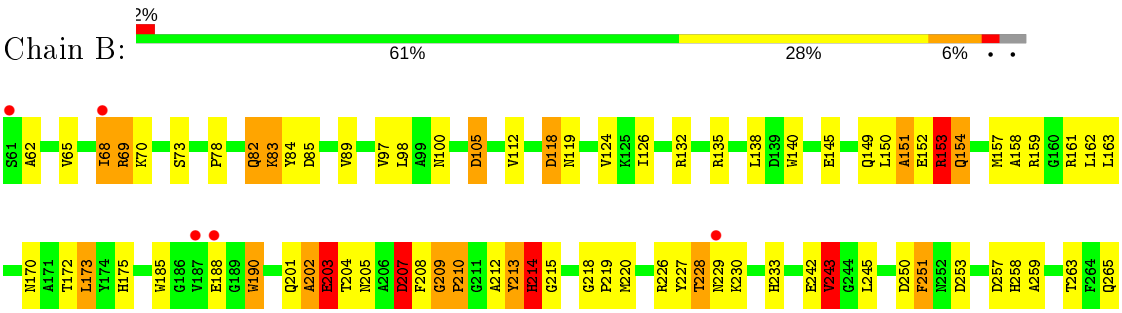
- Molecule 1: Fatty acid Photodecarboxylase

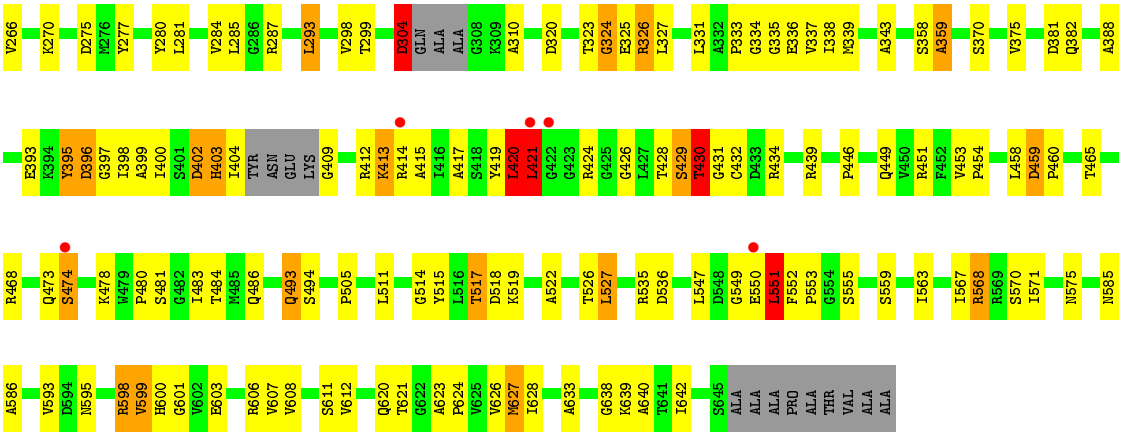
Chain A:



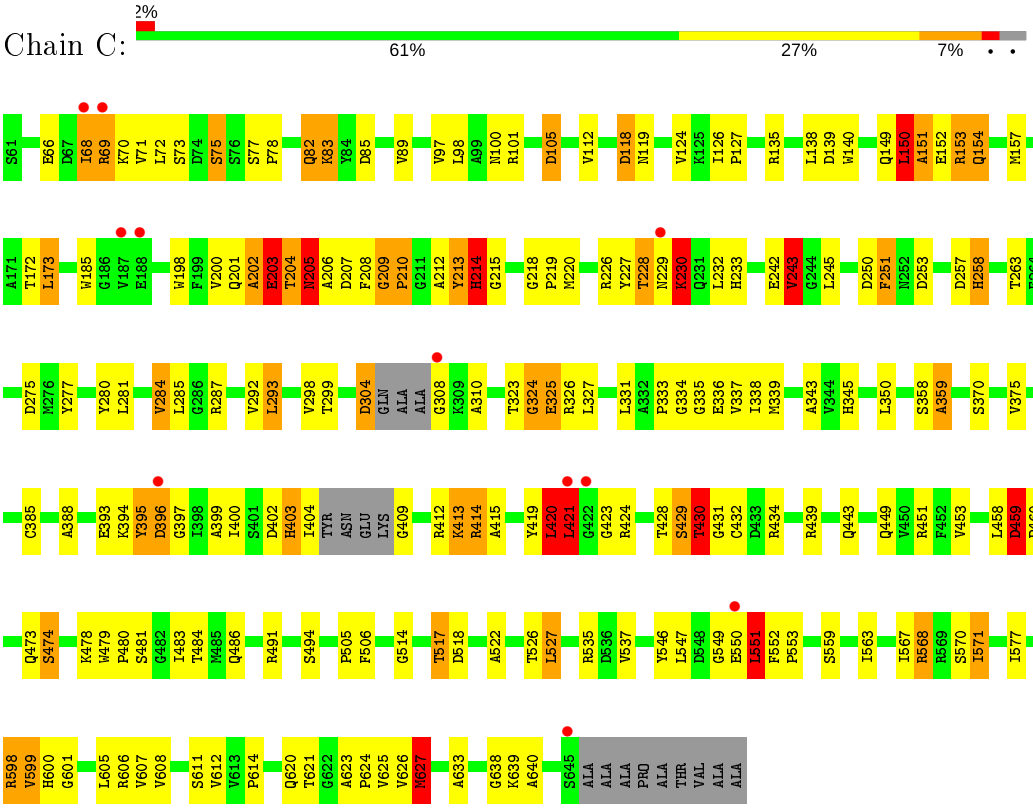
- Molecule 1: Fatty acid Photodecarboxylase

Chain B:

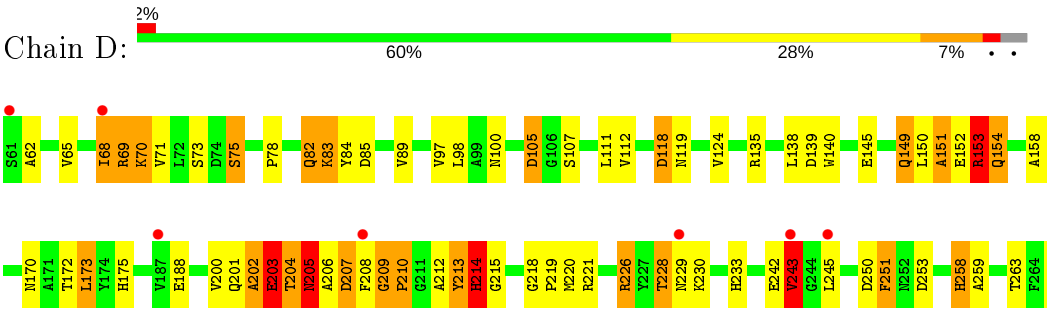


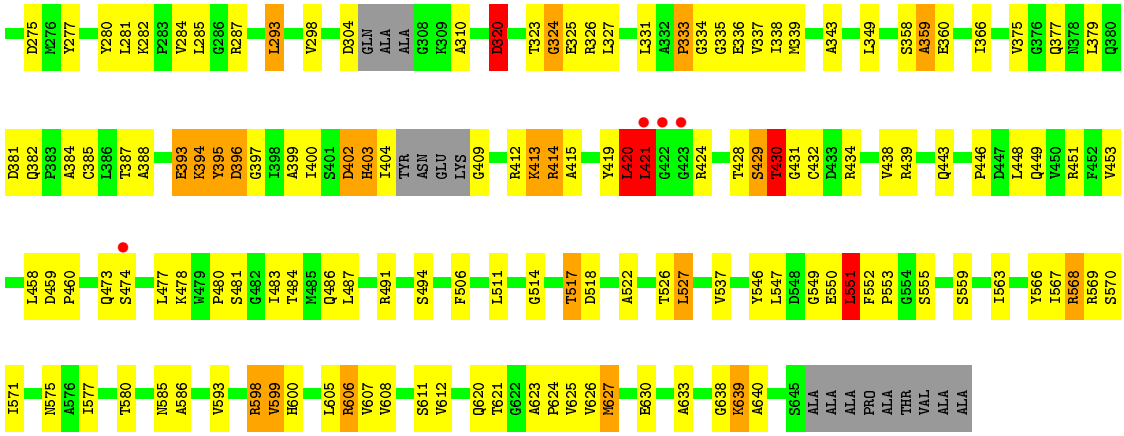


• Molecule 1: Fatty acid Photodecarboxylase



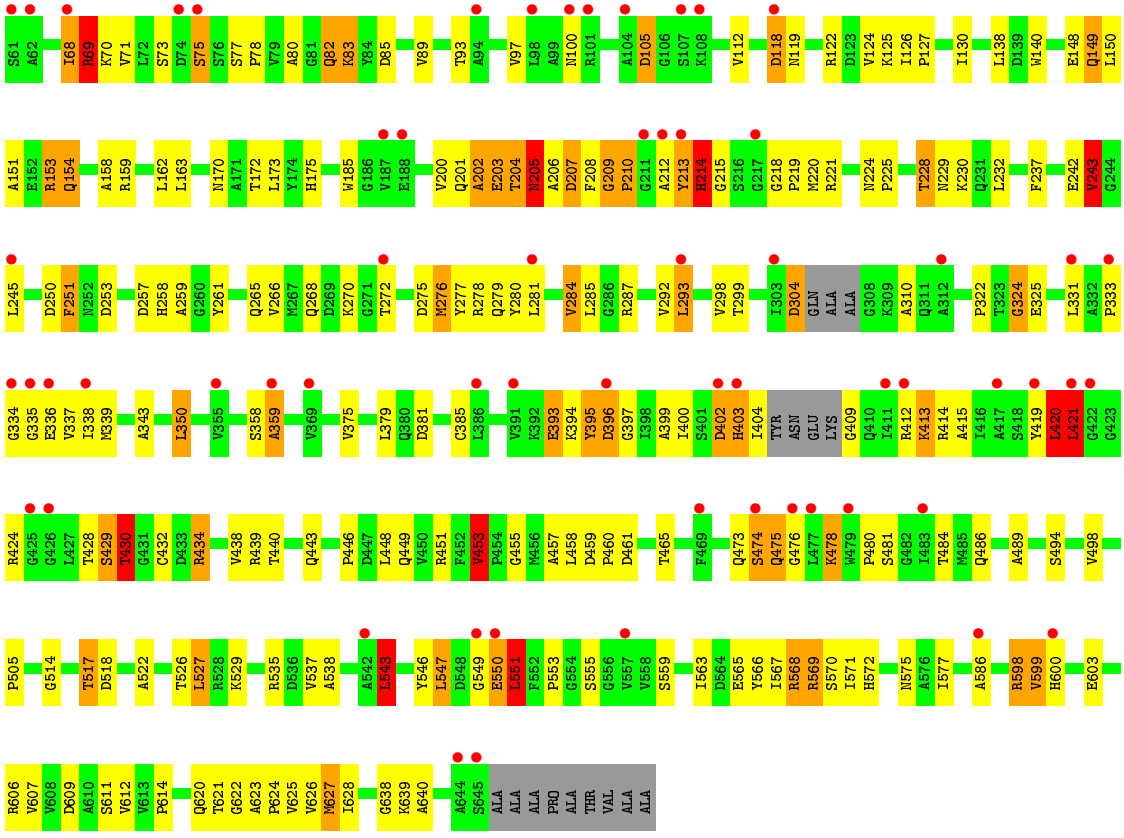
• Molecule 1: Fatty acid Photodecarboxylase





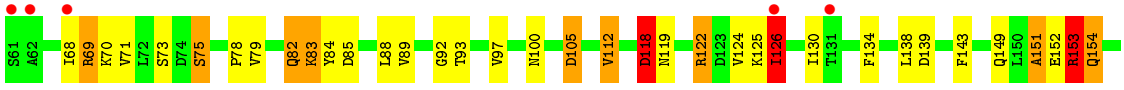
• Molecule 1: Fatty acid Photodecarboxylase

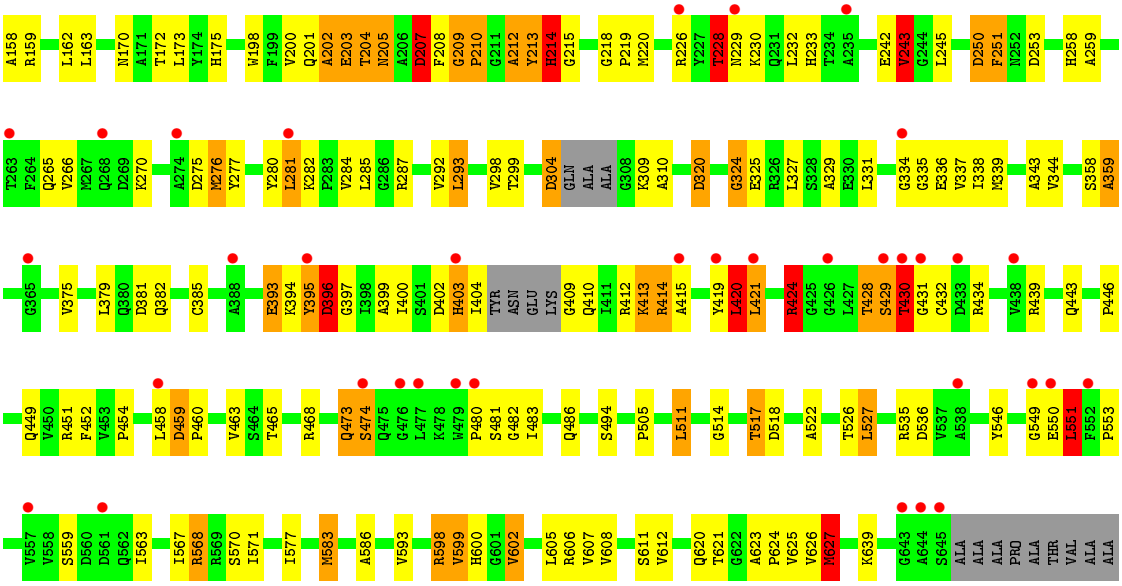
Chain E:



• Molecule 1: Fatty acid Photodecarboxylase

Chain F:




A158 R159 L162 L163 N170 A171 T172 L173 Y174 H175 W198 F199 V200 Q201 A202 E203 T204 N205 A206 D207 F208 G209 P210 G211 A212 Y213 H214 G215 G218 P219 M220 R226 Y227 T228 N229 K230 Q231 L232 H233 T234 A235 E242 V243 G244 L245 D250 F251 N252 D253 H258 A259
T263 F264 Q265 V266 M267 Q268 D269 K270 A274 D275 M276 Y277 Y280 L281 K282 P283 V284 L285 G286 R287 V292 L293 V298 T299 D304 GLN ALA ALA G308 K309 A310 D320 G324 E325 R326 L327 S328 A329 E330 L331 G334 G335 E336 V337 I338 M339 A343 V344 S358 A359
G365 V375 L379 Q380 D381 Q382 C385 A388 E393 K394 Y395 D396 G397 I398 A399 I400 S401 D402 H403 I404 TYR ASN GLU LYS G409 Q410 T411 R412 K413 R414 A415 Y419 L420 L421 R424 G425 G426 L427 T428 S429 T430 G431 C432 D433 R434 V438 R439 Q443 P446
Q449 V450 R451 F452 V453 P454 L458 D459 P460 V463 S464 T465 R468 Q473 S474 Q475 G476 L477 K478 W479 P480 S481 G482 I483 Q486 S494 P505 L511 G514 T517 D518 A522 T526 L527 R535 D536 V537 A538 V546 G549 E550 L551 F552 P553
V557 V558 S559 D560 D561 Q562 I563 I567 R568 R569 S570 I571 I577 M583 A586 V593 R598 V599 H600 G601 V602 L605 R606 V607 V608 S611 V612 Q620 T621 G622 A623 P624 V625 V626 M627 K639 G643 A644 S645 ALA ALA ALA PRO ALA THR VAL ALA ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.23Å 192.11Å 116.13Å 90.00° 113.28° 90.00°	Depositor
Resolution (Å)	49.07 – 3.12 49.07 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.07-3.12) 97.4 (49.07-3.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.225 , 0.278 0.227 , 0.265	Depositor DCC
R_{free} test set	5575 reflections (8.51%)	wwPDB-VP
Wilson B-factor (Å^2)	60.7	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 42.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.853 for H, K, L 0.147 for H, -K, -H-L	Depositor
Outliers	0 of 65516 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	26184	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.65	0/4383	0.92	11/5943 (0.2%)
1	B	0.64	2/4383 (0.0%)	0.93	13/5943 (0.2%)
1	C	0.63	0/4383	0.95	13/5943 (0.2%)
1	D	0.63	1/4383 (0.0%)	0.96	14/5943 (0.2%)
1	E	0.61	0/4383	0.93	12/5943 (0.2%)
1	F	0.60	0/4383	0.94	15/5943 (0.3%)
All	All	0.63	3/26298 (0.0%)	0.94	78/35658 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	3
All	All	0	12

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	203	GLU	CD-OE2	-5.82	1.19	1.25
1	B	326	ARG	CG-CD	-5.76	1.37	1.51
1	D	207	ASP	CB-CG	5.09	1.62	1.51

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	139	ASP	CB-CG-OD2	-16.25	103.68	118.30
1	D	139	ASP	CB-CG-OD1	13.49	130.44	118.30
1	C	420	LEU	CB-CG-CD2	12.72	132.63	111.00
1	C	150	LEU	CB-CG-CD2	-11.67	91.17	111.00
1	E	421	LEU	CB-CG-CD1	-10.60	92.98	111.00
1	F	420	LEU	CA-CB-CG	10.58	139.64	115.30
1	B	527	LEU	CB-CG-CD1	9.55	127.23	111.00
1	E	547	LEU	CA-CB-CG	8.94	135.87	115.30
1	C	230	LYS	CA-CB-CG	-8.87	93.89	113.40
1	F	424	ARG	CG-CD-NE	8.57	129.81	111.80
1	B	320	ASP	CB-CG-OD1	8.56	126.00	118.30
1	A	421	LEU	CA-CB-CG	8.27	134.31	115.30
1	C	421	LEU	CA-CB-CG	8.09	133.91	115.30
1	C	139	ASP	CB-CG-OD1	7.93	125.44	118.30
1	E	421	LEU	CA-CB-CG	7.89	133.45	115.30
1	D	477	LEU	CB-CG-CD2	7.88	124.40	111.00
1	D	320	ASP	CB-CG-OD1	-7.80	111.28	118.30
1	B	421	LEU	CA-CB-CG	7.68	132.97	115.30
1	F	139	ASP	CB-CG-OD1	7.57	125.12	118.30
1	D	421	LEU	CA-CB-CG	7.51	132.58	115.30
1	C	420	LEU	CB-CG-CD1	-7.33	98.54	111.00
1	C	459	ASP	CB-CG-OD1	7.11	124.70	118.30
1	D	320	ASP	CB-CG-OD2	6.97	124.57	118.30
1	D	477	LEU	CA-CB-CG	6.89	131.15	115.30
1	F	583	MET	CA-CB-CG	6.74	124.77	113.30
1	A	551	LEU	CA-CB-CG	6.71	130.73	115.30
1	D	420	LEU	CA-CB-CG	6.67	130.64	115.30
1	B	326	ARG	NE-CZ-NH1	-6.67	116.97	120.30
1	F	421	LEU	CA-CB-CG	6.63	130.54	115.30
1	B	320	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	551	LEU	CA-CB-CG	6.52	130.30	115.30
1	D	551	LEU	CA-CB-CG	6.52	130.30	115.30
1	A	420	LEU	CA-CB-CG	6.51	130.27	115.30
1	B	551	LEU	CA-CB-CG	6.51	130.27	115.30
1	C	420	LEU	CA-CB-CG	6.49	130.22	115.30
1	E	551	LEU	CA-CB-CG	6.46	130.17	115.30
1	F	551	LEU	CA-CB-CG	6.45	130.14	115.30
1	A	238	LYS	CB-CG-CD	6.38	128.20	111.60
1	E	420	LEU	CA-CB-CG	6.33	129.86	115.30
1	A	293	LEU	CB-CG-CD1	-6.22	100.43	111.00
1	B	420	LEU	CA-CB-CG	6.16	129.46	115.30
1	D	203	GLU	OE1-CD-OE2	-6.08	116.01	123.30
1	B	304	ASP	CB-CG-OD2	5.97	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	453	VAL	CA-CB-CG1	5.96	119.84	110.90
1	F	281	LEU	CA-CB-CG	5.94	128.96	115.30
1	C	350	LEU	CB-CG-CD2	5.88	121.00	111.00
1	A	194	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	221	ARG	CA-CB-CG	5.78	126.12	113.40
1	E	421	LEU	CB-CG-CD2	5.77	120.80	111.00
1	A	207	ASP	CB-CG-OD2	5.73	123.45	118.30
1	D	207	ASP	CB-CG-OD2	5.66	123.40	118.30
1	F	207	ASP	CB-CG-OD2	5.65	123.39	118.30
1	E	543	LEU	CB-CG-CD1	5.57	120.47	111.00
1	E	207	ASP	CB-CG-OD2	5.54	123.29	118.30
1	F	118	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	420	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	F	396	ASP	CB-CG-OD1	-5.37	113.47	118.30
1	F	126	ILE	CA-CB-CG1	5.37	121.19	111.00
1	C	82	GLN	C-N-CA	5.29	134.92	121.70
1	F	511	LEU	CB-CG-CD2	5.29	119.98	111.00
1	B	207	ASP	CB-CG-OD2	5.26	123.04	118.30
1	B	203	GLU	OE1-CD-OE2	-5.25	116.99	123.30
1	F	82	GLN	C-N-CA	5.20	134.69	121.70
1	B	266	VAL	CA-CB-CG2	5.18	118.67	110.90
1	D	212	ALA	C-N-CA	5.16	134.61	121.70
1	C	325	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	C	212	ALA	C-N-CA	5.13	134.53	121.70
1	E	82	GLN	C-N-CA	5.13	134.51	121.70
1	A	82	GLN	C-N-CA	5.12	134.51	121.70
1	F	212	ALA	C-N-CA	5.12	134.49	121.70
1	B	212	ALA	C-N-CA	5.12	134.49	121.70
1	D	606	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	212	ALA	C-N-CA	5.11	134.47	121.70
1	E	212	ALA	C-N-CA	5.09	134.43	121.70
1	B	82	GLN	C-N-CA	5.09	134.42	121.70
1	D	82	GLN	C-N-CA	5.06	134.35	121.70
1	A	238	LYS	CD-CE-NZ	5.01	123.23	111.70
1	E	434	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ASN	Peptide
1	A	608	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	205	ASN	Peptide
1	B	608	VAL	Peptide
1	C	205	ASN	Peptide
1	C	608	VAL	Peptide
1	D	205	ASN	Peptide
1	D	608	VAL	Peptide
1	E	205	ASN	Peptide
1	F	205	ASN	Peptide
1	F	228	THR	Peptide
1	F	608	VAL	Peptide

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	4299	0	4238	169	0
1	B	4299	0	4238	156	1
1	C	4299	0	4238	172	0
1	D	4299	0	4238	171	1
1	E	4299	0	4238	167	0
1	F	4299	0	4238	162	0
2	A	53	0	31	5	0
2	B	53	0	31	4	0
2	C	53	0	31	9	0
2	D	53	0	31	8	0
2	E	53	0	31	7	0
2	F	53	0	31	5	0
3	A	18	0	31	7	0
3	B	18	0	31	4	0
3	C	18	0	31	3	0
3	D	18	0	31	3	0
All	All	26184	0	25738	980	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (980) 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:E:453:VAL:HG12	1:E:484:THR:HB	1.26	1.18
1:C:395:TYR:CD1	1:C:478:LYS:NZ	2.12	1.17
1:C:400:ILE:HD11	1:C:481:SER:HB2	1.33	1.08
1:C:400:ILE:HD11	1:C:481:SER:CB	1.83	1.07
1:C:429:SER:HB3	1:C:430:THR:HA	1.38	1.06
1:B:417:ALA:HB1	1:C:421:LEU:HA	1.35	1.05
1:F:429:SER:HB3	1:F:430:THR:HA	1.36	1.05
1:B:397:GLY:H	1:B:400:ILE:HB	1.21	1.04
1:B:400:ILE:HD11	1:B:481:SER:CB	1.86	1.04
1:B:417:ALA:CB	1:C:421:LEU:HA	1.87	1.04
1:A:400:ILE:HD11	1:A:481:SER:HB2	1.40	1.04
1:B:429:SER:HB3	1:B:430:THR:HA	1.39	1.04
1:F:232:LEU:HD13	1:F:483:ILE:HD11	1.35	1.04
1:B:400:ILE:HD11	1:B:481:SER:HB2	1.38	1.03
1:C:397:GLY:H	1:C:400:ILE:HB	1.21	1.03
1:E:429:SER:HB3	1:E:430:THR:HA	1.40	1.03
1:A:421:LEU:CD2	1:D:421:LEU:HG	1.87	1.03
1:A:429:SER:HB3	1:A:430:THR:HA	1.37	1.03
1:F:397:GLY:H	1:F:400:ILE:HB	1.21	1.02
1:D:338:ILE:HG22	1:D:606:ARG:HB2	1.41	1.02
1:A:397:GLY:H	1:A:400:ILE:HB	1.22	1.02
1:A:338:ILE:HG22	1:A:606:ARG:HB2	1.41	1.01
1:D:397:GLY:H	1:D:400:ILE:HB	1.22	1.01
1:B:338:ILE:HG22	1:B:606:ARG:HB2	1.41	1.01
1:E:338:ILE:HG22	1:E:606:ARG:HB2	1.42	1.00
1:D:429:SER:HB3	1:D:430:THR:HA	1.40	1.00
1:E:397:GLY:H	1:E:400:ILE:HB	1.21	0.99
1:F:400:ILE:HD11	1:F:481:SER:HB2	1.42	0.99
1:F:400:ILE:HD11	1:F:481:SER:CB	1.93	0.98
1:C:338:ILE:HG22	1:C:606:ARG:HB2	1.43	0.98
1:D:400:ILE:HD11	1:D:481:SER:HB2	1.44	0.97
1:A:400:ILE:HD11	1:A:481:SER:CB	1.93	0.97
1:D:400:ILE:HD11	1:D:481:SER:CB	1.94	0.96
1:F:126:ILE:HD12	1:F:419:TYR:CE1	2.02	0.93
1:F:338:ILE:HG22	1:F:606:ARG:HB2	1.51	0.91
1:E:158:ALA:O	1:E:159:ARG:HD2	1.73	0.89
1:A:158:ALA:O	1:A:159:ARG:HD2	1.74	0.88
1:D:158:ALA:O	1:D:159:ARG:HD2	1.73	0.87
1:F:429:SER:CB	1:F:430:THR:HA	2.05	0.87
1:B:158:ALA:O	1:B:159:ARG:HD2	1.73	0.87
1:F:158:ALA:O	1:F:159:ARG:HD2	1.73	0.87
1:A:421:LEU:HD22	1:D:421:LEU:HG	1.58	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:SER:CB	1:A:430:THR:HA	2.05	0.86
1:E:486:GLN:HE21	1:E:572:HIS:HE1	1.23	0.86
1:B:429:SER:CB	1:B:430:THR:HA	2.06	0.85
1:C:429:SER:CB	1:C:430:THR:HA	2.05	0.85
1:F:454:PRO:HA	1:F:483:ILE:HD12	1.59	0.84
1:B:335:GLY:HA3	1:B:336:GLU:HB2	1.59	0.84
1:C:400:ILE:HD11	1:C:481:SER:OG	1.78	0.84
1:D:429:SER:CB	1:D:430:THR:HA	2.06	0.84
1:A:421:LEU:HD21	1:D:421:LEU:HG	1.58	0.84
1:A:335:GLY:HA3	1:A:336:GLU:HB2	1.61	0.83
1:E:429:SER:CB	1:E:430:THR:HA	2.07	0.83
1:C:620:GLN:HB2	2:C:701:FAD:C2	2.08	0.83
1:B:400:ILE:HD11	1:B:481:SER:OG	1.78	0.83
1:F:212:ALA:HB3	1:F:213:TYR:CD2	2.14	0.83
1:E:335:GLY:HA3	1:E:336:GLU:HB2	1.60	0.83
1:C:153:ARG:HA	1:C:154:GLN:HB2	1.61	0.83
1:E:153:ARG:HA	1:E:154:GLN:HB2	1.61	0.82
1:F:412:ARG:HB3	1:F:413:LYS:O	1.78	0.82
1:C:400:ILE:CD1	1:C:481:SER:OG	2.27	0.82
1:D:420:LEU:H	1:D:424:ARG:HD2	1.45	0.82
1:C:412:ARG:HB3	1:C:413:LYS:O	1.80	0.82
1:B:400:ILE:CD1	1:B:481:SER:OG	2.28	0.82
1:B:153:ARG:HA	1:B:154:GLN:HB2	1.61	0.81
1:E:453:VAL:CG1	1:E:484:THR:HB	2.08	0.81
1:F:153:ARG:HA	1:F:154:GLN:HB2	1.62	0.81
1:D:412:ARG:HB3	1:D:413:LYS:O	1.79	0.81
1:A:153:ARG:HA	1:A:154:GLN:HB2	1.61	0.81
1:B:412:ARG:HB3	1:B:413:LYS:O	1.81	0.81
1:E:400:ILE:HD11	1:E:481:SER:HB2	1.61	0.80
1:C:420:LEU:H	1:C:424:ARG:HD2	1.45	0.80
1:E:420:LEU:H	1:E:424:ARG:HD2	1.45	0.80
1:E:412:ARG:HB3	1:E:413:LYS:O	1.81	0.80
1:D:335:GLY:HA3	1:D:336:GLU:HB2	1.61	0.79
1:F:134:PHE:CD2	1:F:463:VAL:HG13	2.17	0.79
1:B:420:LEU:H	1:B:424:ARG:HD2	1.46	0.79
1:F:429:SER:HB3	1:F:430:THR:CA	2.11	0.79
1:B:170:ASN:HB3	1:B:172:THR:H	1.48	0.79
1:E:400:ILE:HD11	1:E:481:SER:CB	2.12	0.79
1:A:420:LEU:H	1:A:424:ARG:HD2	1.46	0.79
1:C:335:GLY:HA3	1:C:336:GLU:HB2	1.62	0.79
1:A:429:SER:HB3	1:A:430:THR:CA	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:SER:HB3	1:B:430:THR:CA	2.13	0.78
1:D:170:ASN:HB3	1:D:172:THR:H	1.48	0.78
1:D:153:ARG:HA	1:D:154:GLN:HB2	1.62	0.78
1:F:212:ALA:CB	1:F:213:TYR:HD2	1.96	0.78
1:E:429:SER:HB3	1:E:430:THR:CA	2.12	0.78
1:E:170:ASN:HB3	1:E:172:THR:H	1.48	0.78
1:A:385:CYS:SG	1:A:527:LEU:HD23	2.23	0.78
1:A:170:ASN:HB3	1:A:172:THR:H	1.48	0.78
1:E:130:ILE:HG21	1:E:430:THR:CG2	2.14	0.78
1:F:400:ILE:HD11	1:F:481:SER:OG	1.84	0.77
1:D:400:ILE:HD11	1:D:481:SER:OG	1.84	0.77
1:B:299:THR:HG21	1:B:326:ARG:NH1	1.98	0.77
1:C:429:SER:HB3	1:C:430:THR:CA	2.12	0.76
1:F:335:GLY:HA3	1:F:336:GLU:HB2	1.66	0.76
1:F:420:LEU:O	1:F:421:LEU:HG	1.86	0.76
1:B:190:TRP:CZ3	1:B:642:ILE:HG21	2.20	0.76
1:B:190:TRP:HZ3	1:B:642:ILE:HG21	1.48	0.76
1:C:170:ASN:HB3	1:C:172:THR:H	1.48	0.76
1:F:170:ASN:HB3	1:F:172:THR:H	1.49	0.76
1:A:620:GLN:HB2	2:A:701:FAD:C2	2.15	0.76
1:D:400:ILE:CD1	1:D:481:SER:OG	2.34	0.76
1:F:454:PRO:HA	1:F:483:ILE:CD1	2.15	0.76
1:C:598:ARG:O	1:C:599:VAL:HB	1.87	0.75
1:C:453:VAL:HG21	3:C:702:PLM:H72	1.68	0.75
1:F:79:VAL:HG23	1:F:84:TYR:CE2	2.22	0.74
1:F:88:LEU:HB2	1:F:112:VAL:HG13	1.68	0.74
1:D:598:ARG:O	1:D:599:VAL:HB	1.87	0.74
1:F:598:ARG:O	1:F:599:VAL:HB	1.87	0.74
1:E:77:SER:OG	1:E:80:ALA:HB2	1.86	0.74
1:F:232:LEU:HD13	1:F:483:ILE:CD1	2.14	0.74
1:E:453:VAL:HG12	1:E:484:THR:CB	2.14	0.74
1:A:412:ARG:HB3	1:A:413:LYS:O	1.87	0.73
1:F:396:ASP:HA	1:F:400:ILE:HG21	1.71	0.73
1:E:598:ARG:O	1:E:599:VAL:HB	1.87	0.73
1:D:396:ASP:HA	1:D:400:ILE:HG21	1.71	0.73
1:F:599:VAL:HG13	1:F:602:VAL:HG13	1.70	0.73
1:C:396:ASP:HA	1:C:400:ILE:HG21	1.71	0.72
1:E:396:ASP:HA	1:E:400:ILE:HG21	1.71	0.72
1:A:65:VAL:O	1:A:69:ARG:HG2	1.90	0.72
1:A:598:ARG:O	1:A:599:VAL:HB	1.87	0.72
1:F:400:ILE:CD1	1:F:481:SER:OG	2.36	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:459:ASP:CG	1:C:468:ARG:HH21	1.92	0.72
1:E:567:ILE:O	1:E:568:ARG:HB3	1.89	0.72
1:F:79:VAL:HG23	1:F:84:TYR:HE2	1.55	0.71
1:B:598:ARG:O	1:B:599:VAL:HB	1.88	0.71
1:D:567:ILE:O	1:D:568:ARG:HB3	1.90	0.71
1:C:625:VAL:HG21	2:C:701:FAD:H5'2	1.73	0.71
1:A:396:ASP:HA	1:A:400:ILE:HG21	1.72	0.71
1:A:400:ILE:HD11	1:A:481:SER:OG	1.89	0.70
1:B:396:ASP:HA	1:B:400:ILE:HG21	1.71	0.70
1:C:567:ILE:O	1:C:568:ARG:HB3	1.91	0.70
1:D:429:SER:HB3	1:D:430:THR:CA	2.14	0.70
1:E:228:THR:HA	1:E:434:ARG:NH2	2.07	0.70
1:D:336:GLU:OE2	1:D:598:ARG:NH1	2.24	0.70
1:B:567:ILE:O	1:B:568:ARG:HB3	1.90	0.69
1:D:385:CYS:SG	1:D:527:LEU:HD23	2.32	0.69
1:F:567:ILE:O	1:F:568:ARG:HB3	1.92	0.69
1:E:486:GLN:HE21	1:E:572:HIS:CE1	2.09	0.69
1:A:567:ILE:O	1:A:568:ARG:HB3	1.92	0.69
1:F:226:ARG:HE	1:F:270:LYS:HD3	1.57	0.68
1:F:97:VAL:HG21	1:F:626:VAL:HG13	1.74	0.68
1:D:397:GLY:N	1:D:400:ILE:HB	2.04	0.68
1:C:230:LYS:HG2	1:C:232:LEU:H	1.59	0.68
1:A:400:ILE:CD1	1:A:481:SER:OG	2.41	0.68
1:B:417:ALA:HB1	1:C:421:LEU:CA	2.20	0.68
1:B:209:GLY:H	1:B:210:PRO:HD2	1.57	0.68
1:D:484:THR:HG21	3:D:702:PLM:H81	1.76	0.67
1:E:404:ILE:HG13	1:E:409:GLY:N	2.09	0.67
1:A:458:LEU:HD21	1:A:480:PRO:HG2	1.77	0.67
1:F:394:LYS:HE3	1:F:546:TYR:CD1	2.30	0.67
1:E:458:LEU:HD21	1:E:480:PRO:HG2	1.77	0.67
1:D:233:HIS:ND1	1:D:434:ARG:HD2	2.10	0.67
1:C:82:GLN:HA	1:C:83:LYS:HG2	1.76	0.67
1:B:451:ARG:NH2	3:B:702:PLM:H21	2.10	0.67
1:B:458:LEU:HD21	1:B:480:PRO:HG2	1.77	0.67
1:C:304:ASP:HB3	1:C:310:ALA:HA	1.77	0.67
1:D:209:GLY:H	1:D:210:PRO:HD2	1.59	0.67
1:C:458:LEU:HD21	1:C:480:PRO:HG2	1.76	0.66
1:F:420:LEU:H	1:F:424:ARG:HD3	1.60	0.66
1:D:277:TYR:CE1	1:D:282:LYS:HB2	2.31	0.66
1:C:209:GLY:H	1:C:210:PRO:HD2	1.59	0.66
1:F:126:ILE:HD12	1:F:419:TYR:HE1	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:209:GLY:H	1:E:210:PRO:HD2	1.58	0.66
1:D:458:LEU:HD21	1:D:480:PRO:HG2	1.77	0.66
1:F:209:GLY:H	1:F:210:PRO:HD2	1.59	0.66
1:F:625:VAL:HG21	2:F:701:FAD:H5'2	1.77	0.66
1:F:230:LYS:NZ	1:F:397:GLY:HA3	2.11	0.65
1:B:230:LYS:NZ	1:B:397:GLY:HA3	2.10	0.65
1:A:126:ILE:HG22	1:A:419:TYR:CE1	2.32	0.65
1:C:150:LEU:HD21	1:C:571:ILE:CG2	2.26	0.65
1:F:226:ARG:HB2	1:F:428:THR:HG21	1.77	0.65
1:B:397:GLY:N	1:B:400:ILE:HB	2.04	0.65
1:E:400:ILE:HD11	1:E:481:SER:OG	1.96	0.65
1:B:620:GLN:HB2	2:B:701:FAD:C2	2.26	0.65
1:B:429:SER:CB	1:B:430:THR:CA	2.75	0.65
1:A:209:GLY:H	1:A:210:PRO:HD2	1.61	0.65
1:C:151:ALA:O	1:C:152:GLU:HG2	1.97	0.65
1:F:379:LEU:HD11	1:F:577:ILE:HD11	1.79	0.65
1:C:395:TYR:CG	1:C:478:LYS:NZ	2.64	0.64
1:A:567:ILE:O	1:A:568:ARG:CB	2.45	0.64
1:A:483:ILE:HG12	1:A:547:LEU:HD21	1.79	0.64
1:C:567:ILE:O	1:C:568:ARG:CB	2.46	0.64
1:D:430:THR:OG1	1:D:431:GLY:N	2.31	0.64
1:B:522:ALA:O	1:B:526:THR:HG22	1.98	0.64
1:C:323:THR:OG1	1:D:135:ARG:NH2	2.26	0.64
1:E:522:ALA:O	1:E:526:THR:HG22	1.98	0.64
1:E:82:GLN:HA	1:E:83:LYS:HB2	1.79	0.64
1:F:429:SER:CB	1:F:430:THR:CA	2.74	0.64
1:F:92:GLY:HA3	2:F:701:FAD:O5B	1.98	0.64
1:D:151:ALA:O	1:D:152:GLU:HG2	1.96	0.64
1:E:429:SER:CB	1:E:430:THR:CA	2.75	0.64
1:A:230:LYS:NZ	1:A:397:GLY:HA3	2.11	0.64
1:C:483:ILE:HG12	1:C:547:LEU:HD21	1.79	0.64
1:E:620:GLN:HB2	2:E:701:FAD:C2	2.27	0.64
1:B:567:ILE:O	1:B:568:ARG:CB	2.45	0.64
1:C:397:GLY:N	1:C:400:ILE:HB	2.04	0.64
1:D:567:ILE:O	1:D:568:ARG:CB	2.45	0.64
1:F:567:ILE:O	1:F:568:ARG:CB	2.46	0.64
1:A:323:THR:OG1	1:B:135:ARG:NH2	2.31	0.63
1:A:304:ASP:HB3	1:A:310:ALA:HA	1.80	0.63
1:A:82:GLN:HA	1:A:83:LYS:HB2	1.80	0.63
1:E:304:ASP:HB3	1:E:310:ALA:HA	1.80	0.63
1:A:429:SER:CB	1:A:430:THR:CA	2.75	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LYS:NZ	1:D:397:GLY:HA3	2.12	0.63
1:F:397:GLY:N	1:F:400:ILE:HB	2.04	0.63
1:F:396:ASP:N	1:F:400:ILE:HD13	2.14	0.63
1:F:430:THR:OG1	1:F:431:GLY:N	2.31	0.63
1:A:397:GLY:N	1:A:400:ILE:HB	2.05	0.63
1:B:82:GLN:HA	1:B:83:LYS:HB2	1.80	0.63
1:E:230:LYS:NZ	1:E:397:GLY:HA3	2.12	0.63
1:A:396:ASP:N	1:A:400:ILE:HD13	2.14	0.63
1:D:304:ASP:HB3	1:D:310:ALA:HA	1.79	0.63
1:C:430:THR:OG1	1:C:431:GLY:N	2.31	0.63
1:D:522:ALA:O	1:D:526:THR:HG22	1.99	0.63
1:B:430:THR:OG1	1:B:431:GLY:N	2.31	0.63
1:E:567:ILE:O	1:E:568:ARG:CB	2.46	0.63
1:C:522:ALA:O	1:C:526:THR:HG22	1.99	0.62
1:A:403:HIS:O	1:A:404:ILE:HG22	1.98	0.62
1:A:522:ALA:O	1:A:526:THR:HG22	2.00	0.62
1:C:135:ARG:NH2	1:D:323:THR:OG1	2.31	0.62
1:A:173:LEU:HB2	2:A:701:FAD:O4	1.99	0.62
1:C:396:ASP:N	1:C:400:ILE:HD13	2.14	0.62
1:B:97:VAL:HG21	1:B:626:VAL:HG13	1.82	0.62
1:D:396:ASP:N	1:D:400:ILE:HD13	2.15	0.62
1:B:483:ILE:HG12	1:B:547:LEU:HD21	1.80	0.62
1:D:483:ILE:HG12	1:D:547:LEU:HD21	1.81	0.62
1:D:82:GLN:HA	1:D:83:LYS:HB2	1.80	0.62
1:E:278:ARG:HD3	1:E:279:GLN:NE2	2.15	0.62
1:A:421:LEU:HD22	1:D:421:LEU:CG	2.28	0.62
1:B:465:THR:HG21	3:B:702:PLM:H91	1.80	0.62
1:E:397:GLY:N	1:E:400:ILE:HB	2.05	0.62
1:F:393:GLU:OE2	1:F:395:TYR:HE2	1.81	0.62
1:F:522:ALA:O	1:F:526:THR:HG22	1.99	0.62
1:D:514:GLY:O	1:D:517:THR:HB	2.00	0.62
1:B:514:GLY:O	1:B:517:THR:HB	1.99	0.61
1:F:82:GLN:HA	1:F:83:LYS:HB2	1.82	0.61
1:D:228:THR:O	1:D:230:LYS:N	2.34	0.61
1:E:514:GLY:O	1:E:517:THR:HB	2.00	0.61
1:F:228:THR:O	1:F:230:LYS:N	2.34	0.61
1:B:396:ASP:N	1:B:400:ILE:HD13	2.15	0.61
1:C:420:LEU:O	1:C:421:LEU:HB3	2.00	0.61
1:E:393:GLU:OE2	1:E:395:TYR:HE2	1.83	0.61
1:E:440:THR:HB	1:E:529:LYS:HG2	1.83	0.61
1:C:403:HIS:O	1:C:404:ILE:HG22	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:514:GLY:O	1:F:517:THR:HB	2.00	0.61
1:B:304:ASP:HB3	1:B:310:ALA:HA	1.81	0.61
1:C:514:GLY:O	1:C:517:THR:HB	2.01	0.61
1:D:620:GLN:HB2	2:D:701:FAD:C2	2.30	0.60
1:F:118:ASP:HB2	1:F:163:LEU:HD12	1.83	0.60
1:B:188:GLU:HB2	1:B:585:ASN:HD22	1.65	0.60
1:C:228:THR:O	1:C:230:LYS:N	2.34	0.60
1:E:420:LEU:O	1:E:421:LEU:HB3	2.01	0.60
1:F:403:HIS:O	1:F:404:ILE:HG22	2.01	0.60
1:A:402:ASP:HA	1:A:412:ARG:HG3	1.83	0.60
1:D:403:HIS:O	1:D:404:ILE:HG22	2.01	0.60
1:E:140:TRP:HE1	2:E:701:FAD:H2B	1.66	0.60
1:A:228:THR:O	1:A:230:LYS:N	2.34	0.60
1:B:228:THR:O	1:B:230:LYS:N	2.34	0.60
1:B:62:ALA:HB3	1:B:65:VAL:HG22	1.82	0.60
1:A:514:GLY:O	1:A:517:THR:HB	2.00	0.60
1:E:396:ASP:N	1:E:400:ILE:HD13	2.16	0.60
1:D:97:VAL:HG21	1:D:626:VAL:HG13	1.83	0.60
1:A:62:ALA:HB3	1:A:65:VAL:HG22	1.82	0.60
1:E:228:THR:O	1:E:230:LYS:N	2.34	0.59
1:E:97:VAL:HG21	1:E:626:VAL:HG13	1.83	0.59
1:D:173:LEU:HB2	2:D:701:FAD:O4	2.02	0.59
1:D:429:SER:CB	1:D:430:THR:CA	2.75	0.59
1:E:338:ILE:CG2	1:E:606:ARG:HB2	2.27	0.59
1:F:212:ALA:CB	1:F:213:TYR:CD2	2.76	0.59
1:B:339:MET:HB2	1:B:607:VAL:HG12	1.83	0.59
1:C:230:LYS:HD3	1:C:232:LEU:HB2	1.84	0.59
1:E:230:LYS:HZ1	1:E:397:GLY:HA3	1.67	0.59
1:B:403:HIS:O	1:B:404:ILE:HG22	2.01	0.59
1:F:134:PHE:CE2	1:F:463:VAL:HG13	2.37	0.59
1:B:331:LEU:HD11	1:B:337:VAL:HG23	1.85	0.59
1:E:598:ARG:HH22	1:E:603:GLU:HG2	1.67	0.59
1:F:304:ASP:HB3	1:F:310:ALA:HA	1.83	0.59
1:C:118:ASP:HB2	1:C:163:LEU:HD12	1.84	0.59
1:D:420:LEU:O	1:D:421:LEU:HB3	2.02	0.58
1:F:344:VAL:HG13	1:F:511:LEU:HD21	1.83	0.58
1:A:420:LEU:O	1:A:421:LEU:HB3	2.03	0.58
1:A:430:THR:OG1	1:A:431:GLY:N	2.37	0.58
1:A:575:ASN:HB3	2:A:701:FAD:C8	2.33	0.58
1:C:429:SER:CB	1:C:430:THR:CA	2.75	0.58
1:D:175:HIS:HD2	1:D:620:GLN:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:ASP:HB2	1:D:163:LEU:HD12	1.86	0.58
1:D:62:ALA:HB3	1:D:65:VAL:HG22	1.86	0.58
1:C:77:SER:HB2	1:C:327:LEU:CD2	2.34	0.58
1:B:118:ASP:HB2	1:B:163:LEU:HD12	1.86	0.58
1:B:484:THR:HG21	3:B:702:PLM:H81	1.86	0.58
1:E:403:HIS:O	1:E:404:ILE:HG22	2.03	0.58
1:B:420:LEU:O	1:B:421:LEU:HB3	2.02	0.58
1:C:412:ARG:HA	1:C:413:LYS:HB2	1.85	0.58
1:F:385:CYS:SG	1:F:527:LEU:HD23	2.44	0.58
1:C:331:LEU:HD11	1:C:337:VAL:HG23	1.85	0.58
1:C:620:GLN:HB2	2:C:701:FAD:O2	2.02	0.58
1:E:118:ASP:HB2	1:E:163:LEU:HD12	1.85	0.58
1:B:459:ASP:OD1	1:B:468:ARG:NH2	2.36	0.58
1:C:379:LEU:HD11	1:C:577:ILE:HD11	1.86	0.57
1:E:331:LEU:HD11	1:E:337:VAL:HG23	1.85	0.57
1:A:379:LEU:HD11	1:A:577:ILE:CG2	2.35	0.57
1:F:276:MET:HE3	1:F:280:TYR:CD2	2.40	0.57
1:F:79:VAL:CG2	1:F:84:TYR:HE2	2.16	0.57
1:A:68:ILE:O	1:A:69:ARG:HB3	2.03	0.57
1:E:461:ASP:HA	1:E:572:HIS:CD2	2.39	0.57
1:A:118:ASP:HB2	1:A:163:LEU:HD12	1.87	0.57
1:D:404:ILE:HG13	1:D:409:GLY:N	2.20	0.57
1:A:331:LEU:HD11	1:A:337:VAL:HG23	1.87	0.56
1:A:466:TYR:CE1	3:A:702:PLM:H92	2.40	0.56
1:A:69:ARG:O	1:A:73:SER:HB3	2.06	0.56
1:B:150:LEU:HA	1:B:568:ARG:HG3	1.87	0.56
1:A:97:VAL:HG21	1:A:626:VAL:HG13	1.87	0.56
1:B:202:ALA:HB1	1:B:220:MET:HB2	1.87	0.56
1:D:331:LEU:HD11	1:D:337:VAL:HG23	1.86	0.56
1:D:625:VAL:HG21	2:D:701:FAD:H5'2	1.87	0.56
1:B:343:ALA:HA	1:B:611:SER:HB3	1.87	0.56
1:E:228:THR:HA	1:E:434:ARG:HH21	1.68	0.56
1:E:625:VAL:HG21	2:E:701:FAD:H5'2	1.88	0.56
1:F:69:ARG:O	1:F:73:SER:HB3	2.06	0.56
1:A:233:HIS:ND1	1:A:434:ARG:HD2	2.21	0.56
1:D:623:ALA:HB3	1:D:624:PRO:HD3	1.88	0.56
1:C:219:PRO:HG2	1:C:280:TYR:CZ	2.41	0.55
1:F:331:LEU:HD11	1:F:337:VAL:HG23	1.86	0.55
1:E:623:ALA:HB3	1:E:624:PRO:HD3	1.88	0.55
1:F:324:GLY:O	1:F:325:GLU:HG2	2.05	0.55
1:A:202:ALA:HA	1:A:218:GLY:HA3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:MET:HB2	1:C:607:VAL:HG12	1.89	0.55
1:F:458:LEU:HB3	1:F:468:ARG:HH21	1.70	0.55
1:E:69:ARG:O	1:E:73:SER:HB2	2.06	0.55
1:C:385:CYS:SG	1:C:527:LEU:HD23	2.46	0.55
1:A:219:PRO:HG2	1:A:280:TYR:CZ	2.41	0.55
1:C:623:ALA:HB3	1:C:624:PRO:HD3	1.89	0.55
1:C:69:ARG:O	1:C:73:SER:HB3	2.05	0.55
1:E:339:MET:HG3	1:E:350:LEU:HD11	1.89	0.55
1:A:202:ALA:HB1	1:A:220:MET:HB2	1.88	0.55
1:F:623:ALA:HB3	1:F:624:PRO:HD3	1.89	0.55
1:B:69:ARG:O	1:B:73:SER:HB3	2.06	0.55
1:C:205:ASN:HD22	1:C:206:ALA:H	1.54	0.55
1:B:219:PRO:HG2	1:B:280:TYR:CZ	2.42	0.54
1:D:78:PRO:HG2	1:D:293:LEU:HD21	1.89	0.54
1:D:393:GLU:OE2	1:D:395:TYR:HE2	1.91	0.54
1:D:69:ARG:O	1:D:73:SER:HB3	2.06	0.54
1:F:219:PRO:HG2	1:F:280:TYR:CZ	2.43	0.54
1:F:410:GLN:HG3	1:F:474:SER:H	1.72	0.54
1:F:459:ASP:OD1	1:F:468:ARG:NH2	2.39	0.54
1:C:82:GLN:HA	1:C:83:LYS:CG	2.37	0.54
1:E:400:ILE:CD1	1:E:481:SER:OG	2.55	0.54
1:F:339:MET:HB2	1:F:607:VAL:HG12	1.90	0.54
1:A:623:ALA:HB3	1:A:624:PRO:HD3	1.88	0.54
1:C:202:ALA:HA	1:C:218:GLY:HA3	1.89	0.54
1:C:71:VAL:O	1:C:75:SER:HB3	2.08	0.54
1:E:432:CYS:H	1:E:453:VAL:HG23	1.73	0.54
1:D:575:ASN:HB3	2:D:701:FAD:C8	2.37	0.54
1:E:412:ARG:HA	1:E:413:LYS:HB2	1.89	0.54
1:C:343:ALA:HA	1:C:611:SER:HB3	1.89	0.54
1:F:202:ALA:HA	1:F:218:GLY:HA3	1.89	0.54
1:F:324:GLY:O	1:F:325:GLU:CG	2.56	0.54
1:F:620:GLN:HB2	2:F:701:FAD:C2	2.38	0.54
1:D:202:ALA:HA	1:D:218:GLY:HA3	1.90	0.54
1:D:202:ALA:HB1	1:D:220:MET:HB2	1.90	0.54
1:D:205:ASN:HD22	1:D:206:ALA:H	1.56	0.54
1:A:484:THR:HG21	3:A:702:PLM:H81	1.90	0.54
1:B:78:PRO:HG2	1:B:293:LEU:HD21	1.90	0.54
1:D:68:ILE:O	1:D:69:ARG:HB3	2.08	0.54
1:F:551:LEU:HB2	1:F:553:PRO:HD2	1.90	0.54
1:A:559:SER:O	1:A:563:ILE:HG12	2.09	0.53
1:C:78:PRO:HG2	1:C:293:LEU:HD21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:ALA:H	1:B:65:VAL:HG22	1.73	0.53
1:E:205:ASN:HD22	1:E:206:ALA:H	1.55	0.53
1:E:551:LEU:HB2	1:E:553:PRO:HD2	1.90	0.53
1:A:71:VAL:O	1:A:75:SER:HB3	2.09	0.53
1:B:559:SER:O	1:B:563:ILE:HG12	2.09	0.53
1:B:623:ALA:HB3	1:B:624:PRO:HD3	1.89	0.53
1:D:71:VAL:O	1:D:75:SER:HB3	2.08	0.53
1:A:150:LEU:HA	1:A:568:ARG:HG3	1.89	0.53
1:E:379:LEU:HD13	1:E:498:VAL:HG23	1.90	0.53
1:C:77:SER:HB2	1:C:327:LEU:HD22	1.89	0.53
1:D:219:PRO:HG2	1:D:280:TYR:CZ	2.43	0.53
1:A:343:ALA:HA	1:A:611:SER:HB3	1.90	0.53
1:C:227:TYR:OH	1:C:230:LYS:NZ	2.41	0.53
1:C:140:TRP:HE1	2:C:701:FAD:H2B	1.73	0.53
1:E:322:PRO:HG2	1:F:143:PHE:CD2	2.44	0.53
1:A:205:ASN:HD22	1:A:206:ALA:H	1.55	0.53
1:A:551:LEU:HB2	1:A:553:PRO:HD2	1.89	0.53
1:A:339:MET:HB2	1:A:607:VAL:HG12	1.90	0.53
1:B:299:THR:HG21	1:B:326:ARG:HH12	1.72	0.53
1:B:551:LEU:HB2	1:B:553:PRO:HD2	1.90	0.53
1:C:126:ILE:HG22	1:C:419:TYR:CE1	2.44	0.53
1:C:559:SER:O	1:C:563:ILE:HG12	2.09	0.53
1:D:551:LEU:HB2	1:D:553:PRO:HD2	1.90	0.53
1:F:78:PRO:HG2	1:F:293:LEU:HD21	1.89	0.53
1:F:71:VAL:O	1:F:75:SER:HB3	2.09	0.53
1:A:432:CYS:HB2	1:A:451:ARG:HB3	1.91	0.53
1:C:551:LEU:HB2	1:C:553:PRO:HD2	1.90	0.53
1:F:299:THR:HG23	1:F:505:PRO:HG3	1.90	0.53
1:D:432:CYS:HB2	1:D:451:ARG:HB3	1.90	0.52
1:E:219:PRO:HG2	1:E:280:TYR:CZ	2.43	0.52
1:E:78:PRO:HG2	1:E:293:LEU:HD21	1.91	0.52
1:B:432:CYS:HB2	1:B:451:ARG:HB3	1.92	0.52
1:C:226:ARG:HB2	1:C:428:THR:HG21	1.90	0.52
1:F:602:VAL:HG22	1:F:605:LEU:HB3	1.91	0.52
1:C:82:GLN:CA	1:C:83:LYS:HG2	2.40	0.52
1:C:82:GLN:CB	1:C:83:LYS:HG2	2.39	0.52
1:D:270:LYS:O	1:D:424:ARG:HG2	2.09	0.52
1:E:202:ALA:HA	1:E:218:GLY:HA3	1.90	0.52
1:E:559:SER:O	1:E:563:ILE:HG12	2.09	0.52
1:B:202:ALA:HA	1:B:218:GLY:HA3	1.91	0.52
1:B:453:VAL:HG21	3:B:702:PLM:H72	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LYS:HE3	1:C:546:TYR:CD1	2.44	0.52
1:D:412:ARG:HA	1:D:413:LYS:HB2	1.92	0.52
1:C:432:CYS:HB2	1:C:451:ARG:HB3	1.92	0.52
1:E:343:ALA:HB3	1:E:577:ILE:HG23	1.91	0.52
1:C:404:ILE:HG13	1:C:409:GLY:N	2.24	0.52
1:C:97:VAL:HG21	1:C:626:VAL:HG13	1.91	0.52
1:D:343:ALA:HA	1:D:611:SER:HB3	1.90	0.52
1:D:559:SER:O	1:D:563:ILE:HG12	2.09	0.52
1:E:130:ILE:HG21	1:E:430:THR:HG21	1.88	0.52
1:E:71:VAL:O	1:E:75:SER:HB3	2.09	0.52
1:C:484:THR:HG21	3:C:702:PLM:H81	1.91	0.52
1:D:119:ASN:HD22	1:D:124:VAL:HG11	1.75	0.52
1:F:226:ARG:NE	1:F:270:LYS:HD3	2.22	0.52
1:D:402:ASP:HA	1:D:412:ARG:HG3	1.90	0.52
1:D:598:ARG:O	1:D:606:ARG:HA	2.10	0.52
1:E:460:PRO:HB2	1:E:570:SER:HB3	1.91	0.52
1:F:432:CYS:HB2	1:F:451:ARG:HB3	1.92	0.52
1:F:559:SER:O	1:F:563:ILE:HG12	2.09	0.52
1:B:119:ASN:HD22	1:B:124:VAL:HG11	1.75	0.52
1:B:598:ARG:O	1:B:606:ARG:HA	2.10	0.52
1:C:202:ALA:HB1	1:C:220:MET:HB2	1.92	0.52
1:D:213:TYR:O	1:D:214:HIS:HB2	2.10	0.52
1:A:198:TRP:HB2	1:A:627:MET:CE	2.41	0.51
1:C:326:ARG:NH2	1:C:506:PHE:HE2	2.09	0.51
1:A:62:ALA:H	1:A:65:VAL:HG22	1.75	0.51
1:C:150:LEU:HA	1:C:568:ARG:HG3	1.92	0.51
1:F:599:VAL:CG1	1:F:602:VAL:HG13	2.38	0.51
1:E:299:THR:HG23	1:E:505:PRO:HG3	1.93	0.51
1:A:465:THR:HG21	3:A:702:PLM:H91	1.93	0.51
1:E:270:LYS:O	1:E:424:ARG:HG2	2.10	0.51
1:A:598:ARG:O	1:A:606:ARG:HA	2.11	0.51
1:A:552:PHE:HA	1:B:68:ILE:HD13	1.93	0.51
1:F:233:HIS:ND1	1:F:434:ARG:HD2	2.25	0.51
1:B:230:LYS:NZ	1:B:396:ASP:O	2.44	0.51
1:D:395:TYR:HB3	1:D:478:LYS:NZ	2.25	0.51
1:E:379:LEU:HD11	1:E:577:ILE:HD11	1.92	0.51
1:C:400:ILE:CD1	1:C:481:SER:CB	2.72	0.51
1:F:343:ALA:HB3	1:F:577:ILE:HG23	1.93	0.51
1:A:230:LYS:NZ	1:A:396:ASP:O	2.44	0.51
1:A:326:ARG:NH2	1:A:506:PHE:HE2	2.09	0.51
1:B:175:HIS:HD2	1:B:620:GLN:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:ARG:HA	1:D:414:ARG:HE	1.76	0.51
1:E:202:ALA:HB1	1:E:220:MET:HB2	1.92	0.51
1:F:203:GLU:OE2	1:F:205:ASN:ND2	2.40	0.51
1:C:598:ARG:O	1:C:606:ARG:HA	2.11	0.51
1:D:62:ALA:H	1:D:65:VAL:HG22	1.74	0.51
1:E:598:ARG:O	1:E:606:ARG:HA	2.11	0.51
1:F:119:ASN:HD22	1:F:124:VAL:HG11	1.76	0.51
1:C:173:LEU:HB2	2:C:701:FAD:O4	2.11	0.51
1:D:449:GLN:HE22	1:D:620:GLN:NE2	2.09	0.51
1:F:202:ALA:HB1	1:F:220:MET:HB2	1.92	0.51
1:F:598:ARG:O	1:F:606:ARG:HA	2.11	0.51
1:D:226:ARG:HD2	1:D:270:LYS:HD2	1.93	0.50
1:D:230:LYS:NZ	1:D:396:ASP:O	2.43	0.50
1:F:250:ASP:N	1:F:250:ASP:OD2	2.44	0.50
1:F:126:ILE:HG23	1:F:419:TYR:CZ	2.46	0.50
1:A:453:VAL:HG21	3:A:702:PLM:C7	2.41	0.50
1:C:413:LYS:HB3	1:C:414:ARG:NH1	2.26	0.50
1:F:325:GLU:O	1:F:325:GLU:HG3	2.11	0.50
1:A:205:ASN:HD21	1:A:265:GLN:NE2	2.09	0.50
1:B:230:LYS:HZ1	1:B:397:GLY:HA3	1.74	0.50
1:C:213:TYR:O	1:C:214:HIS:HB2	2.12	0.50
1:C:552:PHE:HA	1:D:68:ILE:HD13	1.93	0.50
1:F:230:LYS:NZ	1:F:396:ASP:O	2.45	0.50
1:E:119:ASN:HD22	1:E:124:VAL:HG11	1.77	0.50
1:F:449:GLN:HE22	1:F:620:GLN:NE2	2.09	0.50
1:C:449:GLN:HE22	1:C:620:GLN:NE2	2.10	0.50
1:F:213:TYR:O	1:F:214:HIS:HB2	2.12	0.50
1:F:259:ALA:HB2	1:F:446:PRO:HG3	1.94	0.50
1:D:230:LYS:CE	1:D:397:GLY:HA3	2.41	0.50
1:E:209:GLY:H	1:E:210:PRO:CD	2.25	0.50
1:A:466:TYR:HE1	3:A:702:PLM:H92	1.76	0.50
1:E:230:LYS:NZ	1:E:396:ASP:O	2.43	0.50
1:A:449:GLN:HE22	1:A:620:GLN:NE2	2.10	0.49
1:B:230:LYS:CE	1:B:397:GLY:HA3	2.41	0.49
1:D:65:VAL:O	1:D:69:ARG:CG	2.60	0.49
1:E:205:ASN:HD21	1:E:265:GLN:NE2	2.10	0.49
1:B:190:TRP:CH2	1:B:642:ILE:HD13	2.47	0.49
1:B:402:ASP:HA	1:B:412:ARG:HG3	1.93	0.49
1:D:226:ARG:HB2	1:D:428:THR:HG21	1.93	0.49
1:E:566:TYR:HA	1:E:569:ARG:HG2	1.93	0.49
1:E:575:ASN:HB3	2:E:701:FAD:C8	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:ARG:NH2	1:E:603:GLU:HG2	2.28	0.49
1:A:119:ASN:HD22	1:A:124:VAL:HG11	1.76	0.49
1:C:414:ARG:N	1:C:414:ARG:HD3	2.26	0.49
1:E:449:GLN:HE22	1:E:620:GLN:NE2	2.10	0.49
1:A:213:TYR:O	1:A:214:HIS:HB2	2.12	0.49
1:D:388:ALA:O	1:D:552:PHE:N	2.45	0.49
1:A:230:LYS:CE	1:A:397:GLY:HA3	2.42	0.49
1:C:205:ASN:HD21	1:C:265:GLN:NE2	2.09	0.49
1:E:213:TYR:O	1:E:214:HIS:HB2	2.13	0.49
1:E:475:GLN:OE1	1:E:476:GLY:N	2.46	0.49
1:D:98:LEU:HD23	1:D:633:ALA:HB2	1.94	0.49
1:F:79:VAL:HG21	1:F:329:ALA:HA	1.94	0.49
1:A:324:GLY:O	1:A:325:GLU:HB3	2.12	0.49
1:D:460:PRO:HB2	1:D:570:SER:HB2	1.95	0.49
1:F:460:PRO:HB2	1:F:570:SER:HB2	1.95	0.49
1:F:343:ALA:HA	1:F:611:SER:HB3	1.95	0.49
1:B:395:TYR:O	1:B:396:ASP:HB2	2.12	0.49
1:C:172:THR:HB	1:C:266:VAL:HG22	1.95	0.49
1:F:230:LYS:HZ1	1:F:397:GLY:HA3	1.77	0.49
1:A:432:CYS:HB2	1:A:451:ARG:HD3	1.95	0.49
1:B:173:LEU:HB2	2:B:701:FAD:O4	2.12	0.48
1:B:324:GLY:O	1:B:325:GLU:HB3	2.12	0.48
1:E:396:ASP:HA	1:E:400:ILE:CG2	2.42	0.48
1:E:565:GLU:OE1	1:E:565:GLU:HA	2.12	0.48
1:A:338:ILE:CG2	1:A:606:ARG:HB2	2.29	0.48
1:B:396:ASP:HA	1:B:400:ILE:CG2	2.43	0.48
1:B:449:GLN:HE22	1:B:620:GLN:NE2	2.10	0.48
1:E:230:LYS:CE	1:E:397:GLY:HA3	2.42	0.48
1:F:404:ILE:HA	1:F:410:GLN:H	1.78	0.48
1:C:119:ASN:HD22	1:C:124:VAL:HG11	1.78	0.48
1:F:230:LYS:CE	1:F:397:GLY:HA3	2.43	0.48
1:A:157:MET:HE3	1:A:511:LEU:HD22	1.95	0.48
1:C:395:TYR:O	1:C:396:ASP:HB2	2.13	0.48
1:D:324:GLY:O	1:D:325:GLU:HB3	2.14	0.48
1:D:396:ASP:HA	1:D:400:ILE:CG2	2.42	0.48
1:E:394:LYS:HE3	1:E:546:TYR:CD1	2.49	0.48
1:E:77:SER:OG	1:E:80:ALA:CB	2.57	0.48
1:B:213:TYR:O	1:B:214:HIS:HB2	2.14	0.48
1:D:209:GLY:H	1:D:210:PRO:CD	2.26	0.48
1:E:230:LYS:HZ3	1:E:232:LEU:HD23	1.79	0.48
1:E:402:ASP:HA	1:E:412:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:598:ARG:HA	1:E:606:ARG:HG2	1.96	0.48
1:A:385:CYS:HG	1:A:527:LEU:HD23	1.79	0.48
1:B:299:THR:CG2	1:B:326:ARG:NH1	2.74	0.48
1:B:460:PRO:HB2	1:B:570:SER:HB2	1.95	0.48
1:C:324:GLY:O	1:C:325:GLU:HB3	2.13	0.48
1:C:620:GLN:CB	2:C:701:FAD:C2	2.86	0.48
1:D:188:GLU:HB2	1:D:585:ASN:HD22	1.78	0.48
1:D:395:TYR:O	1:D:396:ASP:HB2	2.13	0.48
1:D:339:MET:HB2	1:D:607:VAL:HG12	1.95	0.48
1:B:201:GLN:O	1:B:202:ALA:CB	2.61	0.48
1:B:263:THR:HG23	1:B:434:ARG:HG2	1.94	0.48
1:C:138:LEU:HD22	1:C:162:LEU:HD13	1.95	0.48
1:C:201:GLN:O	1:C:202:ALA:CB	2.62	0.48
1:A:209:GLY:H	1:A:210:PRO:CD	2.27	0.48
1:B:98:LEU:HD23	1:B:633:ALA:HB2	1.95	0.48
1:C:209:GLY:H	1:C:210:PRO:CD	2.26	0.48
1:D:172:THR:HB	1:D:266:VAL:HG22	1.95	0.48
1:A:395:TYR:O	1:A:396:ASP:HB2	2.13	0.48
1:A:598:ARG:HA	1:A:606:ARG:HG2	1.96	0.48
1:E:395:TYR:O	1:E:396:ASP:HB2	2.13	0.48
1:C:459:ASP:OD1	1:C:468:ARG:NH2	2.42	0.48
1:D:453:VAL:HG21	3:D:702:PLM:H71	1.95	0.48
1:F:172:THR:HB	1:F:266:VAL:HG22	1.96	0.48
1:A:172:THR:HB	1:A:266:VAL:HG22	1.96	0.47
1:B:270:LYS:O	1:B:424:ARG:HG2	2.14	0.47
1:B:257:ASP:CG	1:B:439:ARG:HH22	2.16	0.47
1:B:281:LEU:HG	1:B:285:LEU:HD13	1.96	0.47
1:A:421:LEU:HD22	1:D:421:LEU:CD1	2.43	0.47
1:F:395:TYR:O	1:F:396:ASP:HB2	2.14	0.47
1:A:284:VAL:HG13	1:A:287:ARG:HD2	1.97	0.47
1:D:413:LYS:O	1:D:415:ALA:N	2.43	0.47
1:D:65:VAL:O	1:D:69:ARG:HG2	2.14	0.47
1:F:201:GLN:O	1:F:202:ALA:CB	2.62	0.47
1:F:396:ASP:HA	1:F:400:ILE:CG2	2.42	0.47
1:A:205:ASN:HD22	1:A:206:ALA:N	2.12	0.47
1:A:460:PRO:HB2	1:A:570:SER:HB2	1.95	0.47
1:C:281:LEU:HG	1:C:285:LEU:HD13	1.97	0.47
1:F:198:TRP:HB2	1:F:627:MET:HE3	1.95	0.47
1:B:299:THR:CG2	1:B:326:ARG:HH12	2.27	0.47
1:C:205:ASN:HD22	1:C:206:ALA:N	2.12	0.47
1:C:413:LYS:HB3	1:C:414:ARG:CZ	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:MET:CE	1:E:350:LEU:HD13	2.44	0.47
1:E:598:ARG:HH22	1:E:603:GLU:CG	2.27	0.47
1:A:281:LEU:HG	1:A:285:LEU:HD13	1.97	0.47
1:B:598:ARG:HA	1:B:606:ARG:HG2	1.96	0.47
1:C:400:ILE:HD12	1:C:481:SER:OG	2.14	0.47
1:E:68:ILE:O	1:E:69:ARG:HB2	2.15	0.47
1:C:275:ASP:OD1	1:C:277:TYR:HB3	2.15	0.47
1:C:304:ASP:OD2	1:C:308:GLY:N	2.47	0.47
1:D:205:ASN:HD22	1:D:206:ALA:N	2.13	0.47
1:D:207:ASP:CB	1:D:265:GLN:HE22	2.28	0.47
1:D:281:LEU:HG	1:D:285:LEU:HD13	1.96	0.47
1:D:598:ARG:HA	1:D:606:ARG:HG2	1.96	0.47
1:E:150:LEU:HA	1:E:568:ARG:HG3	1.97	0.47
1:E:172:THR:HB	1:E:266:VAL:HG22	1.95	0.47
1:E:201:GLN:O	1:E:202:ALA:CB	2.62	0.47
1:A:263:THR:HG23	1:A:434:ARG:HG2	1.96	0.47
1:C:494:SER:HB2	1:C:517:THR:HG22	1.97	0.47
1:F:275:ASP:OD1	1:F:277:TYR:HB3	2.15	0.47
1:F:482:GLY:O	1:F:483:ILE:HD13	2.14	0.47
1:B:185:TRP:HZ3	1:B:190:TRP:CD1	2.33	0.47
1:B:209:GLY:H	1:B:210:PRO:CD	2.25	0.47
1:B:227:TYR:CD1	1:B:426:GLY:CA	2.98	0.47
1:C:460:PRO:HB2	1:C:570:SER:HB2	1.95	0.47
1:F:151:ALA:O	1:F:152:GLU:HG2	2.15	0.47
1:A:201:GLN:O	1:A:202:ALA:CB	2.62	0.47
1:B:535:ARG:HG2	1:B:551:LEU:HD21	1.96	0.47
1:E:275:ASP:OD1	1:E:277:TYR:HB3	2.15	0.47
1:F:494:SER:HB2	1:F:517:THR:HG22	1.96	0.47
1:A:404:ILE:HG13	1:A:409:GLY:N	2.30	0.46
1:A:412:ARG:HA	1:A:413:LYS:HB3	1.97	0.46
1:C:465:THR:HG21	3:C:702:PLM:H91	1.97	0.46
1:D:138:LEU:HD22	1:D:162:LEU:HD13	1.97	0.46
1:D:201:GLN:O	1:D:202:ALA:CB	2.63	0.46
1:E:432:CYS:HB2	1:E:451:ARG:HB3	1.97	0.46
1:A:147:GLN:HB2	1:A:150:LEU:HB2	1.97	0.46
1:C:153:ARG:HA	1:C:154:GLN:CB	2.41	0.46
1:C:263:THR:HG23	1:C:434:ARG:HG2	1.96	0.46
1:D:394:LYS:HE3	1:D:546:TYR:CD1	2.51	0.46
1:D:243:VAL:HG11	1:D:537:VAL:HG22	1.97	0.46
1:E:175:HIS:HD2	1:E:620:GLN:HG2	1.79	0.46
1:F:122:ARG:HA	1:F:125:LYS:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ASP:HA	1:C:400:ILE:CG2	2.42	0.46
1:D:326:ARG:NH2	1:D:506:PHE:HE2	2.14	0.46
1:F:130:ILE:HG12	1:F:134:PHE:HE1	1.80	0.46
1:F:379:LEU:HD11	1:F:577:ILE:CD1	2.44	0.46
1:F:419:TYR:HA	1:F:424:ARG:HA	1.98	0.46
1:F:598:ARG:HA	1:F:606:ARG:HG2	1.96	0.46
1:A:135:ARG:NH2	1:B:323:THR:OG1	2.42	0.46
1:C:381:ASP:OD1	1:C:381:ASP:O	2.33	0.46
1:C:419:TYR:HA	1:C:424:ARG:HA	1.97	0.46
1:D:175:HIS:HB2	1:D:620:GLN:H	1.80	0.46
1:E:205:ASN:HD22	1:E:206:ALA:N	2.13	0.46
1:E:494:SER:HB2	1:E:517:THR:HG22	1.97	0.46
1:A:535:ARG:HG2	1:A:551:LEU:HD21	1.97	0.46
1:D:275:ASP:OD1	1:D:277:TYR:HB3	2.15	0.46
1:D:284:VAL:HG13	1:D:287:ARG:HD2	1.97	0.46
1:D:379:LEU:HD11	1:D:577:ILE:HD11	1.96	0.46
1:F:138:LEU:HD22	1:F:162:LEU:HD13	1.98	0.46
1:A:157:MET:CE	1:A:511:LEU:HD22	2.45	0.46
1:B:157:MET:CE	1:B:511:LEU:HD22	2.46	0.46
1:B:284:VAL:HG13	1:B:287:ARG:HD2	1.97	0.46
1:B:381:ASP:OD1	1:B:381:ASP:O	2.33	0.46
1:D:349:LEU:HD11	2:D:701:FAD:N6A	2.30	0.46
1:A:126:ILE:HG22	1:A:419:TYR:CZ	2.50	0.46
1:A:419:TYR:HA	1:A:424:ARG:HA	1.98	0.46
1:B:275:ASP:OD1	1:B:277:TYR:HB3	2.15	0.46
1:B:419:TYR:HA	1:B:424:ARG:HA	1.98	0.46
1:B:400:ILE:HD12	1:B:481:SER:OG	2.13	0.46
1:F:439:ARG:HD3	1:F:443:GLN:O	2.16	0.46
1:B:203:GLU:HG3	1:B:215:GLY:H	1.81	0.46
1:D:432:CYS:HB2	1:D:451:ARG:HD2	1.98	0.46
1:D:494:SER:HB2	1:D:517:THR:HG22	1.96	0.46
1:E:395:TYR:CD1	1:E:478:LYS:HE3	2.51	0.46
1:F:404:ILE:HA	1:F:409:GLY:HA3	1.97	0.46
1:A:381:ASP:O	1:A:381:ASP:OD1	2.34	0.46
1:B:259:ALA:HB2	1:B:446:PRO:HG3	1.98	0.46
1:B:468:ARG:O	1:B:468:ARG:HG2	2.16	0.46
2:C:701:FAD:H1'1	2:C:701:FAD:H9	1.73	0.46
1:D:233:HIS:CE1	1:D:434:ARG:HD2	2.50	0.46
1:D:439:ARG:HD3	1:D:443:GLN:O	2.16	0.46
1:E:284:VAL:HG13	1:E:287:ARG:HD2	1.98	0.46
1:E:627:MET:HE3	1:E:628:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLY:O	1:A:289:ASN:ND2	2.48	0.46
1:A:275:ASP:OD1	1:A:277:TYR:HB3	2.15	0.46
1:B:207:ASP:HB3	1:B:265:GLN:HE22	1.80	0.46
1:D:419:TYR:HA	1:D:424:ARG:HA	1.97	0.46
1:E:453:VAL:HG13	1:E:455:GLY:O	2.16	0.46
1:F:198:TRP:HB2	1:F:627:MET:CE	2.46	0.46
1:F:284:VAL:HG13	1:F:287:ARG:HD2	1.97	0.46
1:B:138:LEU:HD22	1:B:162:LEU:HD13	1.98	0.45
1:C:284:VAL:HG13	1:C:287:ARG:HD2	1.97	0.45
1:C:77:SER:CB	1:C:327:LEU:HD22	2.46	0.45
1:D:150:LEU:HA	1:D:568:ARG:HG3	1.98	0.45
1:D:381:ASP:OD1	1:D:381:ASP:O	2.34	0.45
1:E:130:ILE:HG21	1:E:430:THR:HG23	1.96	0.45
1:F:209:GLY:H	1:F:210:PRO:CD	2.26	0.45
1:F:207:ASP:HB3	1:F:265:GLN:HE22	1.81	0.45
1:A:453:VAL:HG21	3:A:702:PLM:H71	1.98	0.45
1:B:145:GLU:HG2	1:B:511:LEU:O	2.16	0.45
1:B:412:ARG:HA	1:B:413:LYS:HB3	1.99	0.45
1:F:105:ASP:C	1:F:105:ASP:OD1	2.54	0.45
1:A:97:VAL:HG13	1:A:280:TYR:CE2	2.51	0.45
1:C:233:HIS:ND1	1:C:434:ARG:HD2	2.31	0.45
1:D:84:TYR:CE2	1:D:111:LEU:HB2	2.51	0.45
1:E:225:PRO:HG2	1:E:434:ARG:NH1	2.30	0.45
1:E:439:ARG:HD3	1:E:443:GLN:O	2.16	0.45
1:F:320:ASP:O	1:F:320:ASP:CG	2.55	0.45
1:F:593:VAL:HG11	1:F:607:VAL:HG22	1.98	0.45
1:A:138:LEU:HD22	1:A:162:LEU:HD13	1.99	0.45
1:A:412:ARG:CB	1:A:413:LYS:O	2.61	0.45
1:A:494:SER:HB2	1:A:517:THR:HG22	1.97	0.45
1:C:593:VAL:HG11	1:C:607:VAL:HG22	1.99	0.45
1:D:97:VAL:HG13	1:D:280:TYR:CE2	2.51	0.45
1:F:126:ILE:CD1	1:F:419:TYR:CE1	2.89	0.45
1:A:198:TRP:HB2	1:A:627:MET:HE3	1.99	0.45
1:C:105:ASP:C	1:C:105:ASP:OD1	2.53	0.45
1:C:439:ARG:HD3	1:C:443:GLN:O	2.16	0.45
1:D:163:LEU:HB3	1:D:277:TYR:HD2	1.82	0.45
1:E:419:TYR:HA	1:E:424:ARG:HA	1.97	0.45
1:F:381:ASP:OD1	1:F:381:ASP:O	2.35	0.45
1:A:396:ASP:HA	1:A:400:ILE:CG2	2.42	0.45
1:A:439:ARG:HD3	1:A:443:GLN:O	2.16	0.45
1:D:100:ASN:HA	1:D:284:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:285:LEU:HD11	1:E:292:VAL:HG11	1.98	0.45
1:E:381:ASP:OD1	1:E:381:ASP:O	2.34	0.45
1:A:68:ILE:HD13	1:B:552:PHE:HA	1.97	0.45
2:B:701:FAD:H1'1	2:B:701:FAD:H9	1.55	0.45
1:E:453:VAL:HG13	1:E:455:GLY:H	1.81	0.45
1:F:79:VAL:HG22	1:F:79:VAL:O	2.17	0.45
1:C:203:GLU:HG3	1:C:215:GLY:H	1.82	0.45
1:C:370:SER:CB	1:C:601:GLY:HA3	2.47	0.45
1:E:237:PHE:HB3	1:E:261:TYR:HE2	1.82	0.45
1:E:607:VAL:HG12	1:E:609:ASP:HB2	1.99	0.45
1:F:620:GLN:HB2	2:F:701:FAD:O2	2.16	0.45
1:B:203:GLU:OE2	1:B:214:HIS:HA	2.17	0.45
1:B:227:TYR:CD1	1:B:426:GLY:HA2	2.51	0.45
1:C:535:ARG:HG2	1:C:551:LEU:HD21	1.99	0.45
1:E:566:TYR:O	1:E:569:ARG:CG	2.65	0.45
1:F:413:LYS:O	1:F:415:ALA:N	2.43	0.45
1:F:549:GLY:O	1:F:551:LEU:N	2.50	0.45
1:A:383:PRO:HB2	1:A:571:ILE:HD11	1.98	0.44
1:C:598:ARG:HA	1:C:606:ARG:HG2	1.98	0.44
1:D:593:VAL:HG11	1:D:607:VAL:HG22	1.98	0.44
1:E:257:ASP:OD1	1:E:439:ARG:NH2	2.51	0.44
1:E:494:SER:HB3	1:E:518:ASP:H	1.82	0.44
1:A:226:ARG:HB3	1:A:428:THR:HG21	2.00	0.44
1:B:494:SER:HB2	1:B:517:THR:HG22	1.97	0.44
1:C:198:TRP:HB2	1:C:627:MET:HE3	1.99	0.44
1:C:150:LEU:HD21	1:C:571:ILE:HG22	1.99	0.44
1:D:384:ALA:HA	1:D:487:LEU:O	2.18	0.44
1:E:281:LEU:HG	1:E:285:LEU:HD13	1.98	0.44
1:B:257:ASP:OD1	1:B:439:ARG:NH2	2.51	0.44
1:D:118:ASP:HA	1:D:163:LEU:HB2	2.00	0.44
1:D:638:GLY:O	1:D:640:ALA:N	2.46	0.44
1:E:324:GLY:O	1:E:325:GLU:HB2	2.17	0.44
1:A:549:GLY:O	1:A:551:LEU:N	2.51	0.44
1:B:100:ASN:HA	1:B:284:VAL:HG11	1.99	0.44
1:C:140:TRP:CD2	1:C:345:HIS:HE1	2.35	0.44
1:C:494:SER:HB3	1:C:518:ASP:H	1.82	0.44
1:D:420:LEU:N	1:D:424:ARG:HD2	2.24	0.44
1:E:259:ALA:HB2	1:E:446:PRO:HG3	1.99	0.44
1:F:118:ASP:HA	1:F:163:LEU:HB2	1.99	0.44
1:F:494:SER:HB3	1:F:518:ASP:H	1.83	0.44
1:A:285:LEU:HD11	1:A:292:VAL:HG11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:VAL:HG11	1:B:607:VAL:HG22	1.99	0.44
1:C:243:VAL:HG11	1:C:537:VAL:HG22	2.00	0.44
1:D:338:ILE:CG2	1:D:606:ARG:HB2	2.30	0.44
1:E:185:TRP:CE2	1:E:614:PRO:HD2	2.52	0.44
1:F:175:HIS:HB2	1:F:620:GLN:H	1.82	0.44
2:F:701:FAD:H9	2:F:701:FAD:H1'1	1.79	0.44
1:A:593:VAL:HG11	1:A:607:VAL:HG22	1.98	0.44
1:C:207:ASP:HB3	1:C:265:GLN:HE22	1.82	0.44
1:C:285:LEU:HD11	1:C:292:VAL:HG11	1.99	0.44
1:E:203:GLU:HG2	1:E:215:GLY:O	2.18	0.44
1:E:243:VAL:HG11	1:E:537:VAL:HG22	2.00	0.44
1:F:153:ARG:HA	1:F:154:GLN:CB	2.42	0.44
1:B:381:ASP:HB3	1:B:515:TYR:HE1	1.83	0.44
1:C:451:ARG:HB2	1:C:486:GLN:HB3	2.00	0.44
1:F:414:ARG:HE	1:F:414:ARG:HA	1.82	0.44
1:F:93:THR:HG23	1:F:276:MET:HG2	1.99	0.44
1:B:549:GLY:O	1:B:551:LEU:N	2.50	0.44
1:D:381:ASP:O	1:D:382:GLN:HG2	2.18	0.44
1:E:200:VAL:HG13	1:E:215:GLY:HA3	1.98	0.44
1:E:207:ASP:HB3	1:E:265:GLN:HE22	1.81	0.44
1:E:385:CYS:SG	1:E:527:LEU:HD23	2.58	0.44
1:A:251:PHE:C	1:A:253:ASP:H	2.22	0.43
1:A:230:LYS:HZ1	1:A:397:GLY:HA3	1.81	0.43
1:A:388:ALA:O	1:A:552:PHE:N	2.52	0.43
1:B:494:SER:HB3	1:B:518:ASP:H	1.83	0.43
1:C:412:ARG:CB	1:C:413:LYS:O	2.61	0.43
1:C:345:HIS:ND1	2:C:701:FAD:H8A	2.33	0.43
1:D:549:GLY:O	1:D:551:LEU:N	2.50	0.43
1:F:203:GLU:HG2	1:F:215:GLY:O	2.17	0.43
1:A:207:ASP:HB3	1:A:265:GLN:HE22	1.82	0.43
1:A:100:ASN:HA	1:A:284:VAL:HG11	2.00	0.43
1:C:549:GLY:O	1:C:551:LEU:N	2.51	0.43
1:F:251:PHE:C	1:F:253:ASP:H	2.22	0.43
1:F:480:PRO:O	1:F:481:SER:HB3	2.18	0.43
1:A:105:ASP:C	1:A:105:ASP:OD1	2.57	0.43
1:A:113:LEU:HD23	1:A:293:LEU:HD12	2.01	0.43
1:A:358:SER:O	1:A:359:ALA:HB3	2.18	0.43
1:A:280:TYR:OH	1:A:630:GLU:OE2	2.31	0.43
1:C:200:VAL:HG13	1:C:215:GLY:HA3	2.00	0.43
1:D:153:ARG:HA	1:D:154:GLN:CB	2.42	0.43
1:D:358:SER:O	1:D:359:ALA:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:LYS:HZ1	1:D:397:GLY:HA3	1.83	0.43
1:E:251:PHE:C	1:E:253:ASP:H	2.21	0.43
1:E:125:LYS:HE2	1:E:272:THR:HG21	1.99	0.43
1:F:100:ASN:HA	1:F:284:VAL:HG11	1.99	0.43
1:B:226:ARG:HB3	1:B:428:THR:HG21	2.01	0.43
1:C:270:LYS:O	1:C:424:ARG:HG2	2.18	0.43
1:D:251:PHE:C	1:D:253:ASP:H	2.22	0.43
1:E:535:ARG:HG2	1:E:551:LEU:HD21	2.00	0.43
1:F:212:ALA:C	1:F:213:TYR:HD2	2.21	0.43
1:F:276:MET:HE3	1:F:280:TYR:HD2	1.84	0.43
1:A:118:ASP:HA	1:A:163:LEU:HB2	2.00	0.43
1:C:118:ASP:HA	1:C:163:LEU:HB2	2.00	0.43
1:D:566:TYR:HA	1:D:569:ARG:NH1	2.33	0.43
1:A:203:GLU:HG2	1:A:215:GLY:O	2.18	0.43
1:A:377:GLN:O	1:A:580:THR:HA	2.19	0.43
1:D:349:LEU:HD21	2:D:701:FAD:N6A	2.33	0.43
1:E:118:ASP:HA	1:E:163:LEU:HB2	1.99	0.43
2:E:701:FAD:H1'1	2:E:701:FAD:H9	1.80	0.43
1:A:565:GLU:HA	1:A:565:GLU:OE1	2.18	0.43
1:B:105:ASP:C	1:B:105:ASP:OD1	2.56	0.43
1:D:494:SER:HB3	1:D:518:ASP:H	1.83	0.43
1:A:494:SER:HB3	1:A:518:ASP:H	1.83	0.43
1:A:140:TRP:HE1	2:A:701:FAD:H2B	1.82	0.43
1:A:453:VAL:HG21	3:A:702:PLM:H72	2.00	0.43
1:B:493:GLN:OE1	1:B:522:ALA:CB	2.66	0.43
1:B:575:ASN:HB3	2:B:701:FAD:C8	2.49	0.43
1:C:251:PHE:C	1:C:253:ASP:H	2.22	0.43
1:B:417:ALA:HB2	1:C:421:LEU:HA	1.85	0.43
1:D:145:GLU:HG2	1:D:511:LEU:O	2.19	0.43
1:D:337:VAL:O	1:D:605:LEU:HA	2.19	0.43
1:C:72:LEU:HD21	1:D:458:LEU:HD22	2.01	0.43
1:A:243:VAL:HG11	1:A:537:VAL:HG22	2.00	0.43
1:B:420:LEU:N	1:B:424:ARG:HD2	2.25	0.43
1:B:190:TRP:CZ3	1:B:595:ASN:O	2.72	0.43
1:C:388:ALA:O	1:C:552:PHE:N	2.52	0.43
1:E:138:LEU:HD22	1:E:162:LEU:HD13	2.00	0.43
1:F:213:TYR:HD1	1:F:253:ASP:HA	1.83	0.43
1:F:451:ARG:HB2	1:F:486:GLN:HB3	2.01	0.43
1:D:200:VAL:HG13	1:D:215:GLY:HA3	2.01	0.43
1:D:451:ARG:HB2	1:D:486:GLN:HB3	2.01	0.43
1:E:489:ALA:HB2	1:E:527:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:549:GLY:O	1:E:551:LEU:N	2.52	0.43
1:F:89:VAL:HG13	1:F:298:VAL:HG21	2.00	0.43
1:A:400:ILE:CD1	1:A:481:SER:CB	2.82	0.42
1:A:552:PHE:HA	1:B:68:ILE:CD1	2.49	0.42
1:B:451:ARG:HB2	1:B:486:GLN:HB3	2.01	0.42
1:B:243:VAL:CG2	1:B:536:ASP:HB3	2.49	0.42
1:C:358:SER:O	1:C:359:ALA:HB3	2.19	0.42
1:E:276:MET:HE2	1:E:280:TYR:CE2	2.54	0.42
1:A:451:ARG:HB2	1:A:486:GLN:HB3	2.01	0.42
1:B:140:TRP:CH2	1:B:161:ARG:NH1	2.87	0.42
1:B:331:LEU:HD22	1:B:336:GLU:H	1.84	0.42
1:D:105:ASP:C	1:D:105:ASP:OD1	2.57	0.42
1:D:259:ALA:HB2	1:D:446:PRO:HG3	2.01	0.42
1:E:268:GLN:HE22	1:E:428:THR:HG23	1.84	0.42
1:E:621:THR:O	1:E:624:PRO:HD2	2.18	0.42
1:F:358:SER:O	1:F:359:ALA:HB3	2.19	0.42
1:A:413:LYS:O	1:A:415:ALA:N	2.43	0.42
1:A:270:LYS:O	1:A:424:ARG:HG2	2.19	0.42
1:B:153:ARG:HA	1:B:154:GLN:CB	2.42	0.42
1:B:226:ARG:HD3	1:B:270:LYS:HD2	2.00	0.42
1:C:413:LYS:O	1:C:415:ALA:N	2.44	0.42
1:D:280:TYR:OH	1:D:630:GLU:OE2	2.27	0.42
1:D:172:THR:O	2:D:701:FAD:N3	2.53	0.42
1:D:453:VAL:HG21	3:D:702:PLM:C7	2.50	0.42
1:A:325:GLU:HG2	1:A:327:LEU:CD1	2.49	0.42
1:B:621:THR:O	1:B:624:PRO:HD2	2.19	0.42
1:C:185:TRP:CE2	1:C:614:PRO:HD2	2.53	0.42
1:C:257:ASP:OD1	1:C:439:ARG:NH2	2.52	0.42
1:D:325:GLU:HG2	1:D:327:LEU:CD1	2.49	0.42
1:E:413:LYS:O	1:E:415:ALA:N	2.44	0.42
1:A:188:GLU:HB2	1:A:585:ASN:HB3	2.02	0.42
1:B:118:ASP:HA	1:B:163:LEU:HB2	2.00	0.42
1:C:198:TRP:HB2	1:C:627:MET:CE	2.49	0.42
1:E:480:PRO:O	1:E:481:SER:HB3	2.19	0.42
1:F:452:PHE:HE1	1:F:483:ILE:HG21	1.84	0.42
1:A:200:VAL:HG13	1:A:215:GLY:HA3	2.00	0.42
1:A:468:ARG:O	1:A:468:ARG:HG3	2.18	0.42
1:B:251:PHE:C	1:B:253:ASP:H	2.22	0.42
1:B:404:ILE:HG13	1:B:409:GLY:N	2.34	0.42
1:C:226:ARG:NH1	1:C:423:GLY:O	2.53	0.42
1:D:387:THR:HA	1:D:553:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:412:ARG:CB	1:D:413:LYS:O	2.61	0.42
1:E:105:ASP:C	1:E:105:ASP:OD1	2.57	0.42
1:E:93:THR:HG23	1:E:276:MET:HG2	2.02	0.42
1:F:243:VAL:CG2	1:F:536:ASP:HB3	2.49	0.42
1:A:89:VAL:HG13	1:A:298:VAL:HG21	2.01	0.42
1:A:331:LEU:HD22	1:A:336:GLU:H	1.85	0.42
1:A:379:LEU:HD11	1:A:577:ILE:HG21	2.02	0.42
1:A:480:PRO:O	1:A:481:SER:HB3	2.19	0.42
1:A:624:PRO:O	1:A:627:MET:HB3	2.20	0.42
1:B:151:ALA:O	1:B:152:GLU:HG3	2.19	0.42
1:A:288:ARG:HH12	1:C:66:GLU:HG3	1.85	0.42
1:E:100:ASN:HA	1:E:284:VAL:HG11	2.01	0.42
1:A:621:THR:O	1:A:624:PRO:HD2	2.19	0.42
1:B:358:SER:O	1:B:359:ALA:HB3	2.19	0.42
1:B:381:ASP:O	1:B:382:GLN:HG2	2.19	0.42
1:B:480:PRO:O	1:B:481:SER:HB3	2.20	0.42
1:C:381:ASP:O	1:C:382:GLN:HG2	2.19	0.42
1:E:207:ASP:CB	1:E:265:GLN:HE22	2.33	0.42
1:E:624:PRO:O	1:E:627:MET:HB3	2.20	0.42
1:F:320:ASP:O	1:F:320:ASP:OD1	2.38	0.42
1:C:126:ILE:HG22	1:C:419:TYR:CZ	2.55	0.42
1:D:89:VAL:HG13	1:D:298:VAL:HG21	2.01	0.42
1:A:207:ASP:CB	1:A:265:GLN:HE22	2.33	0.42
1:C:480:PRO:O	1:C:481:SER:HB3	2.19	0.42
1:D:343:ALA:HB3	1:D:577:ILE:HG23	2.02	0.42
1:D:621:THR:O	1:D:624:PRO:HD2	2.19	0.42
1:E:358:SER:O	1:E:359:ALA:HB3	2.19	0.42
1:F:473:GLN:HG3	1:F:474:SER:N	2.34	0.42
1:A:258:HIS:CE1	1:A:491:ARG:HH22	2.37	0.41
1:B:370:SER:CB	1:B:601:GLY:HA3	2.50	0.41
1:C:207:ASP:CB	1:C:265:GLN:HE22	2.33	0.41
1:C:459:ASP:OD1	1:C:459:ASP:N	2.53	0.41
1:D:258:HIS:CD2	1:D:491:ARG:HH22	2.38	0.41
1:E:438:VAL:HB	1:E:448:LEU:HD23	2.02	0.41
1:F:535:ARG:HG2	1:F:551:LEU:HD21	2.01	0.41
1:F:621:THR:O	1:F:624:PRO:HD2	2.19	0.41
1:A:620:GLN:HB2	2:A:701:FAD:O2	2.20	0.41
1:B:175:HIS:HB2	1:B:620:GLN:H	1.86	0.41
1:B:207:ASP:CB	1:B:265:GLN:HE22	2.34	0.41
1:C:621:THR:O	1:C:624:PRO:HD2	2.20	0.41
1:D:140:TRP:HZ2	2:D:701:FAD:HO2A	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ILE:HG22	1:B:454:PRO:C	2.41	0.41
1:C:468:ARG:HG2	1:C:479:TRP:CH2	2.55	0.41
1:C:624:PRO:O	1:C:627:MET:HB3	2.21	0.41
1:D:624:PRO:O	1:D:627:MET:HB3	2.20	0.41
1:F:624:PRO:O	1:F:627:MET:HB3	2.21	0.41
1:A:126:ILE:HA	1:A:127:PRO:HD3	1.91	0.41
1:B:89:VAL:HG13	1:B:298:VAL:HG21	2.02	0.41
1:B:638:GLY:O	1:B:640:ALA:N	2.46	0.41
1:E:538:ALA:HA	1:E:543:LEU:HD22	2.03	0.41
1:F:200:VAL:HG13	1:F:215:GLY:HA3	2.01	0.41
1:F:285:LEU:HD11	1:F:292:VAL:HG11	2.01	0.41
1:B:299:THR:HG23	1:B:505:PRO:HG3	2.02	0.41
1:C:258:HIS:CE1	1:C:491:ARG:HH22	2.37	0.41
1:E:457:ALA:HA	1:E:465:THR:HG21	2.02	0.41
1:E:620:GLN:HB2	2:E:701:FAD:N3	2.35	0.41
1:F:381:ASP:O	1:F:382:GLN:HG2	2.20	0.41
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.97	0.41
1:C:89:VAL:HG13	1:C:298:VAL:HG21	2.01	0.41
1:D:377:GLN:O	1:D:580:THR:HA	2.21	0.41
1:E:331:LEU:HD22	1:E:336:GLU:H	1.85	0.41
1:F:122:ARG:O	1:F:125:LYS:HG2	2.20	0.41
1:A:326:ARG:HH21	1:A:506:PHE:HE2	1.69	0.41
1:C:77:SER:HB2	1:C:327:LEU:HD21	2.02	0.41
1:D:320:ASP:O	1:D:320:ASP:CG	2.59	0.41
1:E:89:VAL:HG13	1:E:298:VAL:HG21	2.02	0.41
1:E:343:ALA:HA	1:E:611:SER:HB3	2.01	0.41
1:E:175:HIS:HB2	1:E:620:GLN:H	1.85	0.41
1:A:370:SER:CB	1:A:601:GLY:HA3	2.51	0.41
1:C:101:ARG:HB2	1:C:633:ALA:HB1	2.02	0.41
1:D:438:VAL:HB	1:D:448:LEU:HD23	2.02	0.41
1:D:480:PRO:O	1:D:481:SER:HB3	2.21	0.41
1:D:84:TYR:CD2	1:D:111:LEU:HB2	2.56	0.41
1:E:566:TYR:O	1:E:569:ARG:HG2	2.21	0.41
1:F:412:ARG:HA	1:F:413:LYS:HB3	2.03	0.41
1:B:624:PRO:O	1:B:627:MET:HB3	2.20	0.41
1:C:638:GLY:O	1:C:640:ALA:N	2.46	0.41
1:D:598:ARG:HH11	1:D:606:ARG:HH21	1.68	0.41
1:E:335:GLY:HA3	1:E:336:GLU:CB	2.43	0.41
1:A:150:LEU:HD22	1:A:571:ILE:HG21	2.03	0.41
1:A:153:ARG:HA	1:A:154:GLN:CB	2.42	0.41
1:C:98:LEU:HD23	1:C:633:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:ILE:HA	1:E:127:PRO:HD3	1.92	0.41
1:A:98:LEU:HD23	1:A:633:ALA:HB2	2.03	0.41
1:B:233:HIS:ND1	1:B:434:ARG:HD2	2.36	0.41
1:C:100:ASN:HA	1:C:284:VAL:HG11	2.02	0.41
1:C:343:ALA:HB3	1:C:577:ILE:HG23	2.03	0.41
1:C:620:GLN:HB2	2:C:701:FAD:N3	2.34	0.41
1:D:331:LEU:HD22	1:D:336:GLU:H	1.86	0.41
1:D:494:SER:HB3	1:D:517:THR:H	1.86	0.41
1:E:598:ARG:HD3	1:E:606:ARG:CZ	2.50	0.41
1:F:134:PHE:HD2	1:F:463:VAL:HG13	1.79	0.41
1:B:84:TYR:O	1:B:331:LEU:HA	2.21	0.40
1:D:320:ASP:O	1:D:320:ASP:OD1	2.39	0.40
1:E:638:GLY:O	1:E:640:ALA:N	2.46	0.40
1:B:188:GLU:HB3	1:B:595:ASN:OD1	2.21	0.40
1:B:388:ALA:O	1:B:552:PHE:N	2.54	0.40
1:B:627:MET:HE3	1:B:628:ILE:HG13	2.01	0.40
1:C:126:ILE:HA	1:C:127:PRO:HD3	1.93	0.40
1:C:299:THR:HG23	1:C:505:PRO:HG3	2.03	0.40
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.98	0.40
1:A:259:ALA:HB2	1:A:446:PRO:HG3	2.03	0.40
1:B:413:LYS:O	1:B:415:ALA:N	2.43	0.40
1:C:331:LEU:HD22	1:C:336:GLU:H	1.86	0.40
1:C:337:VAL:O	1:C:605:LEU:HA	2.22	0.40
1:C:420:LEU:N	1:C:424:ARG:HD2	2.25	0.40
1:C:68:ILE:HD13	1:D:552:PHE:HA	2.03	0.40
1:D:263:THR:HG23	1:D:434:ARG:HG2	2.03	0.40
1:D:175:HIS:CD2	1:D:620:GLN:HG2	2.53	0.40
1:E:379:LEU:HD13	1:E:498:VAL:CG2	2.50	0.40
1:E:404:ILE:HA	1:E:409:GLY:CA	2.52	0.40
1:E:622:GLY:H	2:E:701:FAD:C2	2.34	0.40
1:F:207:ASP:CB	1:F:265:GLN:HE22	2.35	0.40
1:A:337:VAL:O	1:A:605:LEU:HA	2.22	0.40
1:A:438:VAL:HB	1:A:448:LEU:HD23	2.04	0.40
1:B:126:ILE:HG22	1:B:419:TYR:CE2	2.57	0.40
1:E:126:ILE:HG13	1:E:126:ILE:O	2.22	0.40
1:F:97:VAL:HG13	1:F:280:TYR:CE1	2.57	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:LYS:NZ	1:D:107:SER:O[1_454]	2.04	0.16

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	572/594 (96%)	463 (81%)	65 (11%)	44 (8%)	1	5
1	B	572/594 (96%)	461 (81%)	67 (12%)	44 (8%)	1	5
1	C	572/594 (96%)	464 (81%)	64 (11%)	44 (8%)	1	5
1	D	572/594 (96%)	465 (81%)	63 (11%)	44 (8%)	1	5
1	E	572/594 (96%)	463 (81%)	65 (11%)	44 (8%)	1	5
1	F	572/594 (96%)	466 (82%)	63 (11%)	43 (8%)	1	5
All	All	3432/3564 (96%)	2782 (81%)	387 (11%)	263 (8%)	1	5

All (263) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	83	LYS
1	A	173	LEU
1	A	202	ALA
1	A	229	ASN
1	A	242	GLU
1	A	245	LEU
1	A	251	PHE
1	A	258	HIS
1	A	550	GLU
1	A	551	LEU
1	A	568	ARG
1	A	599	VAL
1	B	83	LYS
1	B	173	LEU
1	B	202	ALA

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Mol	Chain	Res	Type
1	B	229	ASN
1	B	242	GLU
1	B	245	LEU
1	B	251	PHE
1	B	258	HIS
1	B	550	GLU
1	B	568	ARG
1	B	599	VAL
1	C	83	LYS
1	C	173	LEU
1	C	202	ALA
1	C	229	ASN
1	C	242	GLU
1	C	245	LEU
1	C	251	PHE
1	C	258	HIS
1	C	393	GLU
1	C	550	GLU
1	C	568	ARG
1	C	599	VAL
1	C	639	LYS
1	D	83	LYS
1	D	173	LEU
1	D	202	ALA
1	D	229	ASN
1	D	242	GLU
1	D	245	LEU
1	D	251	PHE
1	D	258	HIS
1	D	550	GLU
1	D	568	ARG
1	D	599	VAL
1	D	639	LYS
1	E	83	LYS
1	E	173	LEU
1	E	202	ALA
1	E	229	ASN
1	E	242	GLU
1	E	245	LEU
1	E	251	PHE
1	E	258	HIS
1	E	550	GLU

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Mol	Chain	Res	Type
1	E	568	ARG
1	E	599	VAL
1	F	83	LYS
1	F	173	LEU
1	F	202	ALA
1	F	229	ASN
1	F	242	GLU
1	F	245	LEU
1	F	251	PHE
1	F	258	HIS
1	F	568	ARG
1	F	599	VAL
1	A	69	ARG
1	A	324	GLY
1	A	393	GLU
1	A	396	ASP
1	A	420	LEU
1	A	430	THR
1	A	586	ALA
1	A	598	ARG
1	A	627	MET
1	A	639	LYS
1	B	69	ARG
1	B	208	PHE
1	B	324	GLY
1	B	393	GLU
1	B	420	LEU
1	B	430	THR
1	B	551	LEU
1	B	598	ARG
1	B	627	MET
1	B	639	LYS
1	C	69	ARG
1	C	324	GLY
1	C	420	LEU
1	C	430	THR
1	C	551	LEU
1	C	586	ALA
1	C	598	ARG
1	C	627	MET
1	D	69	ARG
1	D	208	PHE

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Mol	Chain	Res	Type
1	D	324	GLY
1	D	393	GLU
1	D	396	ASP
1	D	420	LEU
1	D	430	THR
1	D	474	SER
1	D	551	LEU
1	D	586	ALA
1	D	598	ARG
1	D	627	MET
1	E	69	ARG
1	E	324	GLY
1	E	393	GLU
1	E	396	ASP
1	E	420	LEU
1	E	430	THR
1	E	551	LEU
1	E	586	ALA
1	E	598	ARG
1	E	627	MET
1	E	639	LYS
1	F	69	ARG
1	F	208	PHE
1	F	324	GLY
1	F	393	GLU
1	F	395	TYR
1	F	430	THR
1	F	550	GLU
1	F	551	LEU
1	F	598	ARG
1	F	627	MET
1	F	639	LYS
1	A	149	GLN
1	A	203	GLU
1	A	204	THR
1	A	208	PHE
1	A	210	PRO
1	A	359	ALA
1	A	395	TYR
1	A	474	SER
1	B	149	GLN
1	B	203	GLU

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Mol	Chain	Res	Type
1	B	210	PRO
1	B	359	ALA
1	B	395	TYR
1	B	396	ASP
1	B	402	ASP
1	B	474	SER
1	B	586	ALA
1	C	149	GLN
1	C	203	GLU
1	C	204	THR
1	C	208	PHE
1	C	210	PRO
1	C	359	ALA
1	C	395	TYR
1	C	396	ASP
1	C	402	ASP
1	C	474	SER
1	D	204	THR
1	D	210	PRO
1	D	334	GLY
1	D	359	ALA
1	D	395	TYR
1	D	402	ASP
1	E	203	GLU
1	E	204	THR
1	E	208	PHE
1	E	210	PRO
1	E	359	ALA
1	E	395	TYR
1	E	402	ASP
1	E	474	SER
1	F	149	GLN
1	F	203	GLU
1	F	204	THR
1	F	210	PRO
1	F	359	ALA
1	F	396	ASP
1	F	402	ASP
1	F	420	LEU
1	F	586	ALA
1	A	151	ALA
1	A	153	ARG

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Mol	Chain	Res	Type
1	A	154	GLN
1	A	334	GLY
1	A	402	ASP
1	A	413	LYS
1	B	151	ALA
1	B	153	ARG
1	B	154	GLN
1	B	204	THR
1	B	214	HIS
1	B	334	GLY
1	B	413	LYS
1	C	151	ALA
1	C	153	ARG
1	C	154	GLN
1	C	214	HIS
1	C	334	GLY
1	C	413	LYS
1	D	149	GLN
1	D	151	ALA
1	D	153	ARG
1	D	154	GLN
1	D	203	GLU
1	D	214	HIS
1	D	413	LYS
1	E	149	GLN
1	E	151	ALA
1	E	153	ARG
1	E	154	GLN
1	E	214	HIS
1	E	334	GLY
1	E	413	LYS
1	F	151	ALA
1	F	153	ARG
1	F	154	GLN
1	F	214	HIS
1	F	334	GLY
1	F	474	SER
1	A	70	LYS
1	A	209	GLY
1	A	214	HIS
1	A	333	PRO
1	A	399	ALA

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Mol	Chain	Res	Type
1	A	600	HIS
1	B	70	LYS
1	B	333	PRO
1	B	600	HIS
1	C	70	LYS
1	C	600	HIS
1	D	70	LYS
1	D	600	HIS
1	E	70	LYS
1	E	600	HIS
1	F	70	LYS
1	F	399	ALA
1	F	413	LYS
1	F	600	HIS
1	B	209	GLY
1	B	399	ALA
1	C	209	GLY
1	C	333	PRO
1	C	399	ALA
1	D	209	GLY
1	D	399	ALA
1	E	209	GLY
1	E	399	ALA
1	F	209	GLY
1	A	68	ILE
1	B	68	ILE
1	D	68	ILE
1	E	68	ILE
1	E	333	PRO
1	F	68	ILE
1	A	243	VAL
1	B	243	VAL
1	C	68	ILE
1	C	243	VAL
1	D	243	VAL
1	E	243	VAL
1	F	243	VAL
1	D	333	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	446/455 (98%)	405 (91%)	41 (9%)	9 32
1	B	446/455 (98%)	410 (92%)	36 (8%)	11 38
1	C	446/455 (98%)	409 (92%)	37 (8%)	11 37
1	D	446/455 (98%)	406 (91%)	40 (9%)	9 33
1	E	446/455 (98%)	400 (90%)	46 (10%)	7 26
1	F	446/455 (98%)	404 (91%)	42 (9%)	8 32
All	All	2676/2730 (98%)	2434 (91%)	242 (9%)	9 33

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LYS
1	A	75	SER
1	A	85	ASP
1	A	105	ASP
1	A	112	VAL
1	A	118	ASP
1	A	122	ARG
1	A	157	MET
1	A	204	THR
1	A	205	ASN
1	A	213	TYR
1	A	228	THR
1	A	243	VAL
1	A	250	ASP
1	A	284	VAL
1	A	304	ASP
1	A	309	LYS
1	A	320	ASP
1	A	366	ILE
1	A	375	VAL
1	A	393	GLU
1	A	403	HIS

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Mol	Chain	Res	Type
1	A	414	ARG
1	A	420	LEU
1	A	421	LEU
1	A	428	THR
1	A	429	SER
1	A	430	THR
1	A	465	THR
1	A	468	ARG
1	A	473	GLN
1	A	474	SER
1	A	501	LYS
1	A	517	THR
1	A	527	LEU
1	A	550	GLU
1	A	551	LEU
1	A	555	SER
1	A	571	ILE
1	A	612	VAL
1	A	627	MET
1	B	85	ASP
1	B	105	ASP
1	B	112	VAL
1	B	118	ASP
1	B	132	ARG
1	B	153	ARG
1	B	190	TRP
1	B	203	GLU
1	B	207	ASP
1	B	213	TYR
1	B	214	HIS
1	B	228	THR
1	B	243	VAL
1	B	250	ASP
1	B	293	LEU
1	B	304	ASP
1	B	327	LEU
1	B	375	VAL
1	B	403	HIS
1	B	414	ARG
1	B	420	LEU
1	B	421	LEU
1	B	429	SER

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Mol	Chain	Res	Type
1	B	430	THR
1	B	459	ASP
1	B	473	GLN
1	B	474	SER
1	B	478	LYS
1	B	493	GLN
1	B	517	THR
1	B	527	LEU
1	B	551	LEU
1	B	555	SER
1	B	571	ILE
1	B	603	GLU
1	B	612	VAL
1	C	75	SER
1	C	85	ASP
1	C	105	ASP
1	C	112	VAL
1	C	118	ASP
1	C	150	LEU
1	C	157	MET
1	C	203	GLU
1	C	204	THR
1	C	205	ASN
1	C	213	TYR
1	C	214	HIS
1	C	228	THR
1	C	230	LYS
1	C	243	VAL
1	C	250	ASP
1	C	284	VAL
1	C	293	LEU
1	C	304	ASP
1	C	375	VAL
1	C	403	HIS
1	C	414	ARG
1	C	420	LEU
1	C	421	LEU
1	C	429	SER
1	C	430	THR
1	C	459	ASP
1	C	465	THR
1	C	468	ARG

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Mol	Chain	Res	Type
1	C	473	GLN
1	C	474	SER
1	C	517	THR
1	C	527	LEU
1	C	551	LEU
1	C	571	ILE
1	C	612	VAL
1	C	627	MET
1	D	70	LYS
1	D	75	SER
1	D	85	ASP
1	D	105	ASP
1	D	112	VAL
1	D	118	ASP
1	D	149	GLN
1	D	153	ARG
1	D	203	GLU
1	D	204	THR
1	D	205	ASN
1	D	213	TYR
1	D	214	HIS
1	D	221	ARG
1	D	226	ARG
1	D	228	THR
1	D	243	VAL
1	D	250	ASP
1	D	293	LEU
1	D	320	ASP
1	D	333	PRO
1	D	360	GLU
1	D	366	ILE
1	D	375	VAL
1	D	394	LYS
1	D	403	HIS
1	D	414	ARG
1	D	420	LEU
1	D	421	LEU
1	D	429	SER
1	D	430	THR
1	D	459	ASP
1	D	473	GLN
1	D	517	THR

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Mol	Chain	Res	Type
1	D	527	LEU
1	D	551	LEU
1	D	555	SER
1	D	571	ILE
1	D	612	VAL
1	D	639	LYS
1	E	69	ARG
1	E	75	SER
1	E	85	ASP
1	E	105	ASP
1	E	112	VAL
1	E	118	ASP
1	E	122	ARG
1	E	148	GLU
1	E	149	GLN
1	E	204	THR
1	E	205	ASN
1	E	213	TYR
1	E	214	HIS
1	E	221	ARG
1	E	224	ASN
1	E	228	THR
1	E	243	VAL
1	E	250	ASP
1	E	276	MET
1	E	284	VAL
1	E	293	LEU
1	E	304	ASP
1	E	350	LEU
1	E	375	VAL
1	E	403	HIS
1	E	414	ARG
1	E	420	LEU
1	E	421	LEU
1	E	429	SER
1	E	430	THR
1	E	453	VAL
1	E	459	ASP
1	E	473	GLN
1	E	474	SER
1	E	475	GLN
1	E	478	LYS

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Mol	Chain	Res	Type
1	E	517	THR
1	E	527	LEU
1	E	543	LEU
1	E	547	LEU
1	E	550	GLU
1	E	551	LEU
1	E	555	SER
1	E	569	ARG
1	E	571	ILE
1	E	612	VAL
1	F	75	SER
1	F	85	ASP
1	F	105	ASP
1	F	112	VAL
1	F	118	ASP
1	F	122	ARG
1	F	126	ILE
1	F	153	ARG
1	F	204	THR
1	F	207	ASP
1	F	213	TYR
1	F	214	HIS
1	F	228	THR
1	F	243	VAL
1	F	250	ASP
1	F	276	MET
1	F	281	LEU
1	F	282	LYS
1	F	293	LEU
1	F	304	ASP
1	F	309	LYS
1	F	320	ASP
1	F	327	LEU
1	F	375	VAL
1	F	403	HIS
1	F	414	ARG
1	F	420	LEU
1	F	424	ARG
1	F	428	THR
1	F	429	SER
1	F	430	THR
1	F	459	ASP

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Mol	Chain	Res	Type
1	F	465	THR
1	F	473	GLN
1	F	517	THR
1	F	527	LEU
1	F	551	LEU
1	F	571	ILE
1	F	583	MET
1	F	602	VAL
1	F	612	VAL
1	F	627	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	175	HIS
1	A	224	ASN
1	A	265	GLN
1	A	279	GLN
1	A	289	ASN
1	A	352	HIS
1	A	620	GLN
1	B	82	GLN
1	B	119	ASN
1	B	175	HIS
1	B	205	ASN
1	B	224	ASN
1	B	258	HIS
1	B	265	GLN
1	B	585	ASN
1	B	620	GLN
1	C	119	ASN
1	C	224	ASN
1	C	265	GLN
1	C	345	HIS
1	C	352	HIS
1	C	585	ASN
1	C	620	GLN
1	D	175	HIS
1	D	205	ASN
1	D	585	ASN
1	D	620	GLN

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Mol	Chain	Res	Type
1	E	119	ASN
1	E	175	HIS
1	E	265	GLN
1	E	268	GLN
1	E	279	GLN
1	E	352	HIS
1	E	572	HIS
1	E	585	ASN
1	E	620	GLN
1	F	119	ASN
1	F	258	HIS
1	F	265	GLN
1	F	279	GLN
1	F	585	ASN
1	F	620	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

10 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	E	701	-	51,58,58	2.19	10 (19%)	60,89,89	2.10	15 (25%)
2	FAD	B	701	-	51,58,58	2.15	9 (17%)	60,89,89	2.69	22 (36%)
2	FAD	D	701	-	51,58,58	1.79	6 (11%)	60,89,89	2.13	14 (23%)
2	FAD	F	701	-	51,58,58	2.12	8 (15%)	60,89,89	2.18	16 (26%)
3	PLM	D	702	-	14,17,17	0.42	0	13,17,17	0.38	0
3	PLM	B	702	-	14,17,17	0.47	0	13,17,17	0.56	0
3	PLM	C	702	-	14,17,17	0.39	0	13,17,17	0.56	0
2	FAD	A	701	-	51,58,58	2.09	11 (21%)	60,89,89	2.38	14 (23%)
3	PLM	A	702	-	14,17,17	0.45	0	13,17,17	0.51	0
2	FAD	C	701	-	51,58,58	1.99	9 (17%)	60,89,89	2.41	18 (30%)

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	E	701	-	-	7/30/50/50	0/6/6/6
2	FAD	B	701	-	-	13/30/50/50	0/6/6/6
2	FAD	D	701	-	-	15/30/50/50	0/6/6/6
2	FAD	F	701	-	-	16/30/50/50	0/6/6/6
3	PLM	D	702	-	-	9/13/15/15	-
3	PLM	B	702	-	-	9/13/15/15	-
3	PLM	C	702	-	-	10/13/15/15	-
2	FAD	A	701	-	-	10/30/50/50	0/6/6/6
3	PLM	A	702	-	-	8/13/15/15	-
2	FAD	C	701	-	-	7/30/50/50	0/6/6/6

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	701	FAD	C4X-C10	11.89	1.50	1.38
2	B	701	FAD	C4X-C10	11.50	1.50	1.38
2	F	701	FAD	C4X-C10	11.03	1.49	1.38
2	A	701	FAD	C4X-C10	10.31	1.49	1.38
2	C	701	FAD	C4X-C10	9.73	1.48	1.38
2	D	701	FAD	C4X-C10	9.20	1.48	1.38
2	C	701	FAD	C4-C4X	5.09	1.50	1.41
2	D	701	FAD	C4-C4X	4.38	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	FAD	C4-C4X	4.30	1.48	1.41
2	A	701	FAD	C9A-C5X	4.19	1.51	1.42
2	E	701	FAD	C4-C4X	4.16	1.48	1.41
2	F	701	FAD	C9A-N10	3.99	1.43	1.38
2	B	701	FAD	C1'-N10	-3.98	1.44	1.48
2	A	701	FAD	C8-C7	3.95	1.50	1.40
2	F	701	FAD	C8-C7	3.90	1.50	1.40
2	B	701	FAD	C8-C7	3.87	1.50	1.40
2	F	701	FAD	C9A-C5X	3.77	1.50	1.42
2	E	701	FAD	C9A-C5X	3.66	1.49	1.42
2	B	701	FAD	C9A-C5X	3.56	1.49	1.42
2	C	701	FAD	C8-C7	3.47	1.49	1.40
2	E	701	FAD	C8-C7	3.44	1.49	1.40
2	A	701	FAD	C4-C4X	3.35	1.47	1.41
2	E	701	FAD	C10-N1	3.32	1.37	1.33
2	D	701	FAD	C8-C7	3.25	1.49	1.40
2	C	701	FAD	C9A-C5X	3.20	1.49	1.42
2	A	701	FAD	C5A-C4A	3.20	1.49	1.40
2	B	701	FAD	C4-C4X	3.14	1.46	1.41
2	E	701	FAD	C9A-N10	3.09	1.42	1.38
2	A	701	FAD	C9A-N10	2.85	1.42	1.38
2	F	701	FAD	C10-N1	2.77	1.36	1.33
2	A	701	FAD	C1'-N10	-2.76	1.45	1.48
2	E	701	FAD	C5A-C4A	2.61	1.47	1.40
2	D	701	FAD	C9A-C5X	2.58	1.47	1.42
2	A	701	FAD	C2A-N3A	2.52	1.36	1.32
2	C	701	FAD	C2A-N3A	2.47	1.36	1.32
2	D	701	FAD	C2A-N3A	2.43	1.36	1.32
2	C	701	FAD	C4X-N5	2.42	1.36	1.33
2	C	701	FAD	O4B-C1B	2.40	1.44	1.41
2	D	701	FAD	C5A-C4A	2.38	1.47	1.40
2	B	701	FAD	C2B-C1B	-2.37	1.50	1.53
2	B	701	FAD	C5A-C4A	2.37	1.47	1.40
2	E	701	FAD	C4X-N5	2.36	1.36	1.33
2	E	701	FAD	O4B-C1B	2.36	1.44	1.41
2	C	701	FAD	C10-N1	2.33	1.36	1.33
2	F	701	FAD	C5A-C4A	2.32	1.47	1.40
2	B	701	FAD	O3'-C3'	2.26	1.48	1.43
2	F	701	FAD	C2-N3	-2.21	1.33	1.38
2	A	701	FAD	C10-N1	2.16	1.36	1.33
2	A	701	FAD	C6-C5X	-2.11	1.38	1.41
2	B	701	FAD	C2A-N3A	2.11	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C4X-N5	2.04	1.36	1.33
2	E	701	FAD	C2A-N3A	2.04	1.35	1.32
2	C	701	FAD	C1'-N10	-2.00	1.46	1.48

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	FAD	C4-N3-C2	10.90	124.35	115.14
2	A	701	FAD	C4-N3-C2	10.79	124.26	115.14
2	C	701	FAD	C4-N3-C2	9.35	123.04	115.14
2	D	701	FAD	C4-N3-C2	8.97	122.72	115.14
2	E	701	FAD	C4-N3-C2	8.63	122.43	115.14
2	F	701	FAD	C4-N3-C2	8.59	122.39	115.14
2	B	701	FAD	C1'-N10-C10	7.73	125.33	118.41
2	A	701	FAD	C4-C4X-C10	-7.16	115.21	119.95
2	A	701	FAD	C1'-N10-C9A	6.49	123.40	118.29
2	F	701	FAD	C1'-N10-C10	6.02	123.80	118.41
2	C	701	FAD	C4X-N5-C5X	5.99	122.75	116.77
2	C	701	FAD	C4-C4X-C10	-5.95	116.02	119.95
2	E	701	FAD	C4-C4X-C10	-5.44	116.35	119.95
2	B	701	FAD	C4X-C4-N3	-5.43	116.00	123.43
2	F	701	FAD	C4-C4X-C10	-5.34	116.42	119.95
2	C	701	FAD	N3A-C2A-N1A	-5.30	120.39	128.68
2	D	701	FAD	C4X-C4-N3	-5.04	116.54	123.43
2	B	701	FAD	C4'-C3'-C2'	-4.72	103.54	113.36
2	C	701	FAD	C4-C4X-N5	4.71	123.98	118.60
2	D	701	FAD	C1'-N10-C10	4.67	122.59	118.41
2	B	701	FAD	N3A-C2A-N1A	-4.58	121.52	128.68
2	F	701	FAD	C4X-N5-C5X	4.51	121.27	116.77
2	D	701	FAD	C4X-N5-C5X	4.45	121.22	116.77
2	E	701	FAD	C5X-C9A-N10	4.27	120.81	117.72
2	E	701	FAD	P-O3P-PA	-4.16	118.56	132.83
2	B	701	FAD	C5X-C9A-N10	4.08	120.67	117.72
2	F	701	FAD	N3A-C2A-N1A	-4.05	122.34	128.68
2	B	701	FAD	O3'-C3'-C2'	3.82	118.05	108.81
2	A	701	FAD	N3A-C2A-N1A	-3.76	122.81	128.68
2	D	701	FAD	N3A-C2A-N1A	-3.67	122.94	128.68
2	C	701	FAD	C1'-N10-C10	3.63	121.66	118.41
2	E	701	FAD	C4X-N5-C5X	3.61	120.38	116.77
2	B	701	FAD	C4X-N5-C5X	3.53	120.30	116.77
2	A	701	FAD	C4-C4X-N5	3.47	122.56	118.60
2	B	701	FAD	C5'-C4'-C3'	-3.45	105.53	112.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	701	FAD	C4'-C3'-C2'	-3.43	106.23	113.36
2	C	701	FAD	C4X-C4-N3	-3.35	118.86	123.43
2	B	701	FAD	C4-C4X-C10	-3.30	117.77	119.95
2	E	701	FAD	C4X-C4-N3	-3.28	118.95	123.43
2	B	701	FAD	P-O3P-PA	-3.27	121.59	132.83
2	E	701	FAD	N3A-C2A-N1A	-3.26	123.58	128.68
2	A	701	FAD	N6A-C6A-N1A	3.19	125.19	118.57
2	C	701	FAD	P-O3P-PA	-3.18	121.91	132.83
2	E	701	FAD	C1'-N10-C10	3.17	121.25	118.41
2	A	701	FAD	C4X-C4-N3	-3.07	119.24	123.43
2	D	701	FAD	N6A-C6A-N1A	3.04	124.88	118.57
2	B	701	FAD	C9A-N10-C10	-2.93	118.06	121.91
2	F	701	FAD	C5X-C9A-N10	2.93	119.84	117.72
2	B	701	FAD	O4'-C4'-C5'	2.84	116.29	109.92
2	C	701	FAD	C5X-C9A-N10	2.82	119.76	117.72
2	F	701	FAD	C4X-C4-N3	-2.82	119.57	123.43
2	F	701	FAD	C9A-N10-C10	-2.76	118.29	121.91
2	A	701	FAD	C4X-N5-C5X	2.76	119.53	116.77
2	E	701	FAD	C9A-N10-C10	-2.74	118.31	121.91
2	E	701	FAD	C1'-N10-C9A	2.69	120.41	118.29
2	D	701	FAD	C9A-N10-C10	-2.67	118.41	121.91
2	E	701	FAD	C4X-C10-N10	-2.66	117.57	120.30
2	C	701	FAD	O2A-PA-O1A	2.62	125.21	112.24
2	F	701	FAD	C5'-C4'-C3'	-2.62	107.14	112.20
2	B	701	FAD	N6A-C6A-N1A	2.60	123.98	118.57
2	E	701	FAD	C4A-C5A-N7A	-2.59	106.70	109.40
2	C	701	FAD	C5'-C4'-C3'	-2.59	107.21	112.20
2	B	701	FAD	C5A-C6A-N6A	-2.58	116.43	120.35
2	E	701	FAD	O2A-PA-O1A	2.57	124.97	112.24
2	D	701	FAD	C3B-C2B-C1B	2.57	104.85	100.98
2	D	701	FAD	C5'-C4'-C3'	-2.56	107.26	112.20
2	B	701	FAD	O2P-P-O1P	2.56	124.88	112.24
2	D	701	FAD	O3'-C3'-C2'	2.54	114.94	108.81
2	B	701	FAD	O2A-PA-O1A	2.52	124.72	112.24
2	A	701	FAD	O4'-C4'-C5'	-2.52	104.25	109.92
2	C	701	FAD	C6-C5X-N5	2.48	121.78	119.05
2	E	701	FAD	O4B-C1B-C2B	-2.46	103.33	106.93
2	F	701	FAD	O2'-C2'-C3'	2.44	115.03	109.10
2	F	701	FAD	C4X-C10-N10	-2.42	117.81	120.30
2	C	701	FAD	N6A-C6A-N1A	2.38	123.51	118.57
2	C	701	FAD	C2A-N1A-C6A	2.36	122.80	118.75
2	A	701	FAD	C2A-N1A-C6A	2.36	122.78	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	FAD	C9A-N10-C10	-2.34	118.85	121.91
2	A	701	FAD	C1'-C2'-C3'	-2.29	103.38	109.79
2	D	701	FAD	O2'-C2'-C3'	-2.29	103.54	109.10
2	F	701	FAD	C2A-N1A-C6A	2.28	122.66	118.75
2	D	701	FAD	C5A-C6A-N6A	-2.27	116.90	120.35
2	E	701	FAD	C10-C4X-N5	2.26	122.82	121.26
2	B	701	FAD	C4X-C10-N10	-2.24	118.00	120.30
2	B	701	FAD	C1'-N10-C9A	-2.24	116.53	118.29
2	B	701	FAD	C10-C4X-N5	2.24	122.80	121.26
2	F	701	FAD	P-O3P-PA	-2.23	125.17	132.83
2	A	701	FAD	O5'-C5'-C4'	-2.23	103.41	109.36
2	C	701	FAD	O4B-C4B-C3B	2.20	109.48	105.11
2	F	701	FAD	C4-C4X-N5	2.18	121.09	118.60
2	A	701	FAD	C5A-C6A-N6A	-2.18	117.04	120.35
2	D	701	FAD	O4B-C1B-C2B	-2.18	103.74	106.93
2	F	701	FAD	C1B-N9A-C4A	-2.18	122.82	126.64
2	F	701	FAD	N6A-C6A-N1A	2.10	122.94	118.57
2	C	701	FAD	C9A-C5X-N5	-2.09	119.09	122.36
2	B	701	FAD	C8M-C8-C9	-2.09	115.34	120.34
2	B	701	FAD	O5'-P-O1P	-2.09	100.90	109.07
2	C	701	FAD	O2'-C2'-C1'	2.05	114.53	109.59
2	C	701	FAD	C1B-N9A-C4A	-2.03	123.08	126.64

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	701	FAD	C3'-C4'-C5'-O5'
2	E	701	FAD	O4'-C4'-C5'-O5'
2	E	701	FAD	C5'-O5'-P-O1P
2	E	701	FAD	C5'-O5'-P-O2P
2	E	701	FAD	PA-O3P-P-O5'
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A
2	B	701	FAD	C5B-O5B-PA-O3P
2	B	701	FAD	C2'-C1'-N10-C9A
2	B	701	FAD	C2'-C1'-N10-C10
2	B	701	FAD	O4'-C4'-C5'-O5'
2	B	701	FAD	C5'-O5'-P-O1P
2	B	701	FAD	C5'-O5'-P-O2P
2	B	701	FAD	PA-O3P-P-O5'
2	D	701	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	D	701	FAD	C5B-O5B-PA-O3P
2	D	701	FAD	O4'-C4'-C5'-O5'
2	D	701	FAD	C5'-O5'-P-O2P
2	F	701	FAD	C5B-O5B-PA-O1A
2	F	701	FAD	C5B-O5B-PA-O2A
2	F	701	FAD	C5B-O5B-PA-O3P
2	F	701	FAD	C2'-C1'-N10-C9A
2	F	701	FAD	C2'-C1'-N10-C10
2	F	701	FAD	C1'-C2'-C3'-O3'
2	F	701	FAD	C1'-C2'-C3'-C4'
2	F	701	FAD	C5'-O5'-P-O1P
2	F	701	FAD	C5'-O5'-P-O2P
3	C	702	PLM	C1-C2-C3-C4
2	A	701	FAD	C5'-O5'-P-O2P
2	C	701	FAD	C3'-C4'-C5'-O5'
2	C	701	FAD	O4'-C4'-C5'-O5'
2	C	701	FAD	C5'-O5'-P-O3P
2	C	701	FAD	PA-O3P-P-O5'
2	F	701	FAD	O2'-C2'-C3'-O3'
2	B	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	O4B-C4B-C5B-O5B
2	F	701	FAD	C3B-C4B-C5B-O5B
2	A	701	FAD	O4B-C4B-C5B-O5B
2	A	701	FAD	C3B-C4B-C5B-O5B
2	F	701	FAD	O2'-C2'-C3'-C4'
3	A	702	PLM	C6-C7-C8-C9
3	A	702	PLM	CA-CB-CC-CD
3	C	702	PLM	C2-C3-C4-C5
3	B	702	PLM	CA-CB-CC-CD
3	C	702	PLM	C4-C5-C6-C7
3	D	702	PLM	C5-C6-C7-C8
3	D	702	PLM	C9-CA-CB-CC
3	B	702	PLM	C5-C6-C7-C8
3	A	702	PLM	C5-C6-C7-C8
3	D	702	PLM	C2-C3-C4-C5
3	C	702	PLM	CA-CB-CC-CD
3	A	702	PLM	C8-C9-CA-CB
3	D	702	PLM	CA-CB-CC-CD
3	C	702	PLM	CC-CD-CE-CF
3	B	702	PLM	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	B	702	PLM	CB-CC-CD-CE
3	B	702	PLM	C6-C7-C8-C9
3	D	702	PLM	CB-CC-CD-CE
3	D	702	PLM	C6-C7-C8-C9
3	D	702	PLM	C8-C9-CA-CB
3	D	702	PLM	CC-CD-CE-CF
2	B	701	FAD	C3'-C4'-C5'-O5'
3	A	702	PLM	C2-C3-C4-C5
3	C	702	PLM	C5-C6-C7-C8
3	A	702	PLM	C9-CA-CB-CC
2	B	701	FAD	C3B-C4B-C5B-O5B
3	C	702	PLM	CB-CC-CD-CE
3	A	702	PLM	CB-CC-CD-CE
2	E	701	FAD	C5'-O5'-P-O3P
2	D	701	FAD	C5'-O5'-P-O3P
2	A	701	FAD	C5'-O5'-P-O3P
2	D	701	FAD	O2'-C2'-C3'-O3'
2	A	701	FAD	PA-O3P-P-O1P
3	C	702	PLM	C6-C7-C8-C9
2	D	701	FAD	C5B-O5B-PA-O2A
2	D	701	FAD	C5'-O5'-P-O1P
2	A	701	FAD	C5B-O5B-PA-O1A
2	C	701	FAD	C5'-O5'-P-O1P
3	B	702	PLM	C4-C5-C6-C7
2	C	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	P-O3P-PA-O1A
2	D	701	FAD	PA-O3P-P-O2P
2	A	701	FAD	PA-O3P-P-O2P
2	D	701	FAD	O2'-C2'-C3'-C4'
3	B	702	PLM	C8-C9-CA-CB
3	A	702	PLM	C4-C5-C6-C7
3	B	702	PLM	C9-CA-CB-CC
2	A	701	FAD	P-O3P-PA-O1A
2	A	701	FAD	P-O3P-PA-O2A
3	D	702	PLM	C3-C4-C5-C6
2	B	701	FAD	C5'-O5'-P-O3P
2	F	701	FAD	C5'-O5'-P-O3P
2	A	701	FAD	C5B-O5B-PA-O3P
2	E	701	FAD	O4B-C4B-C5B-O5B
2	D	701	FAD	PA-O3P-P-O1P
2	F	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	P-O3P-PA-O2A

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Mol	Chain	Res	Type	Atoms
3	B	702	PLM	CC-CD-CE-CF
2	C	701	FAD	C5B-O5B-PA-O1A
3	C	702	PLM	C8-C9-CA-CB
2	D	701	FAD	C1'-C2'-C3'-O3'
3	C	702	PLM	C9-CA-CB-CC

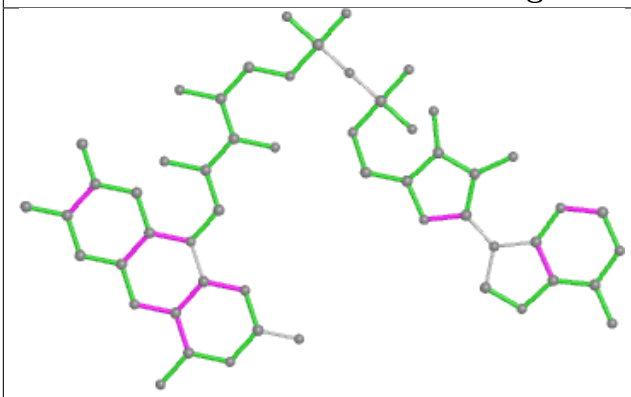
There are no ring outliers.

10 monomers are involved in 55 short contacts:

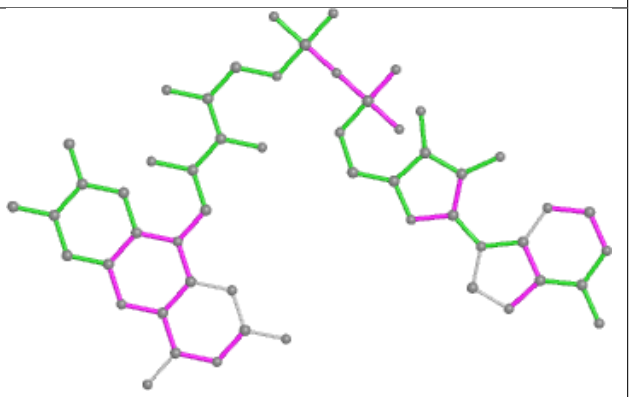
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	701	FAD	7	0
2	B	701	FAD	4	0
2	D	701	FAD	8	0
2	F	701	FAD	5	0
3	D	702	PLM	3	0
3	B	702	PLM	4	0
3	C	702	PLM	3	0
2	A	701	FAD	5	0
3	A	702	PLM	7	0
2	C	701	FAD	9	0

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 then 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.

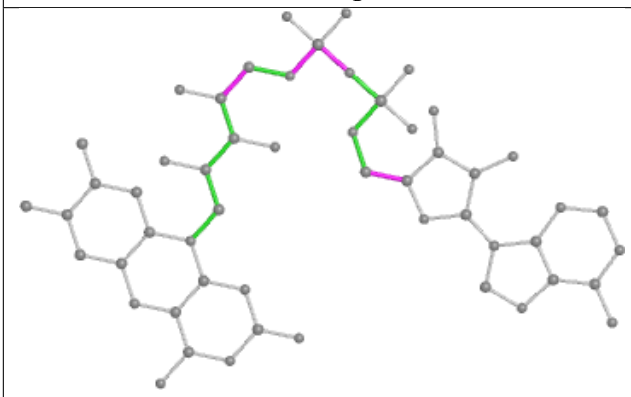
Ligand FAD E 701



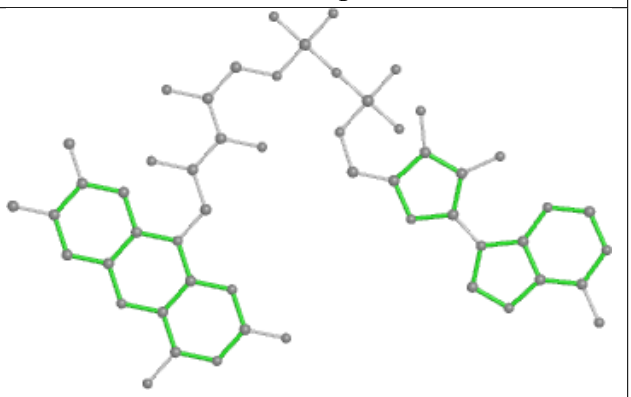
Bond lengths



Bond angles

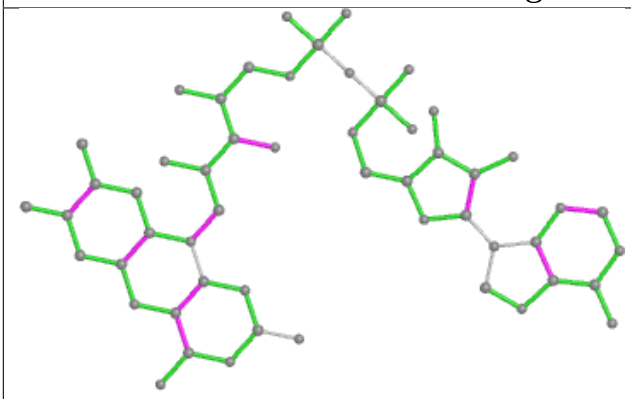


Torsions

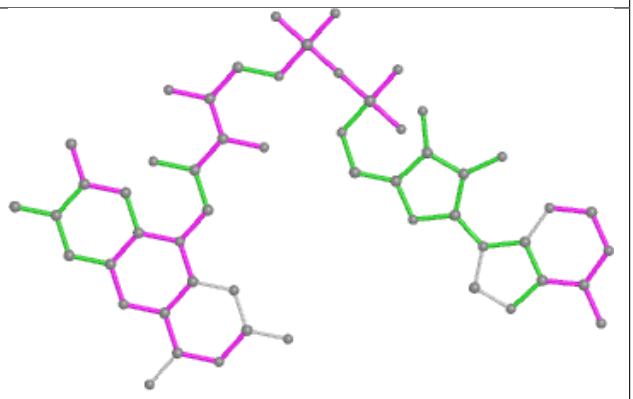


Rings

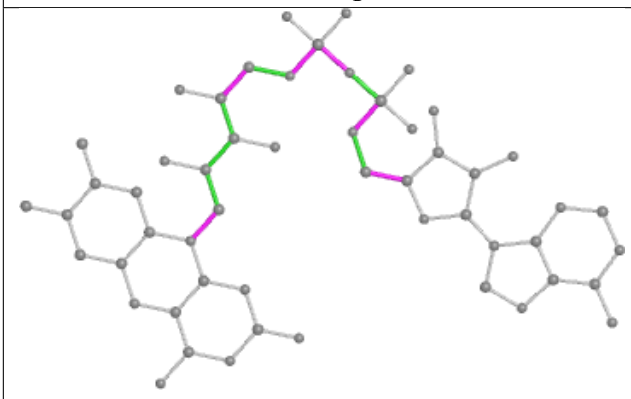
Ligand FAD B 701



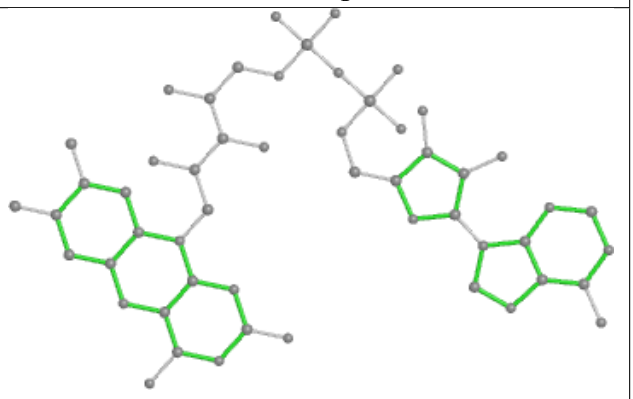
Bond lengths



Bond angles

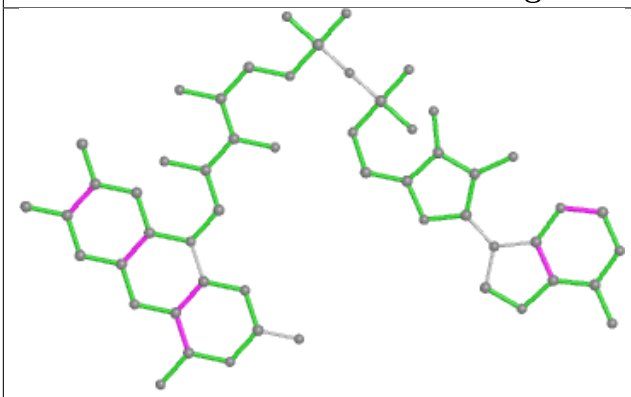


Torsions

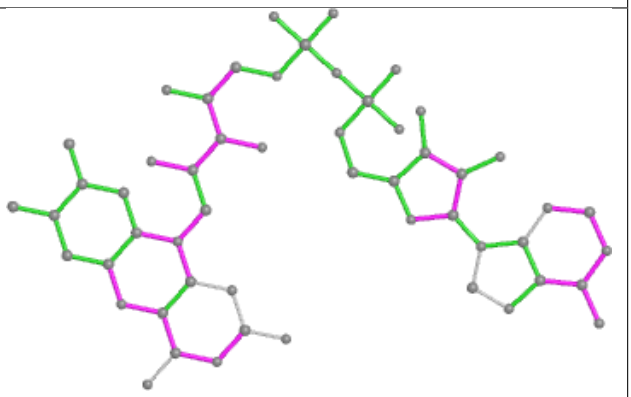


Rings

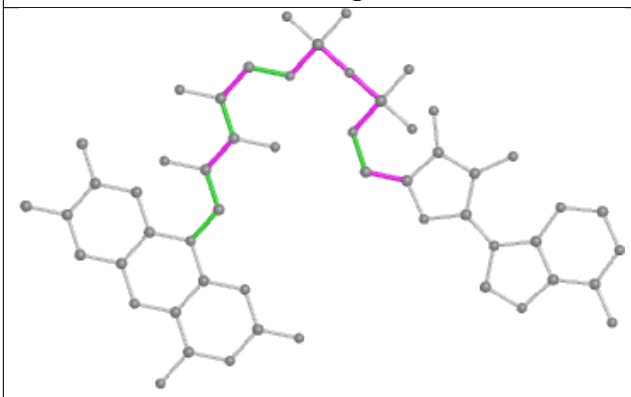
Ligand FAD D 701



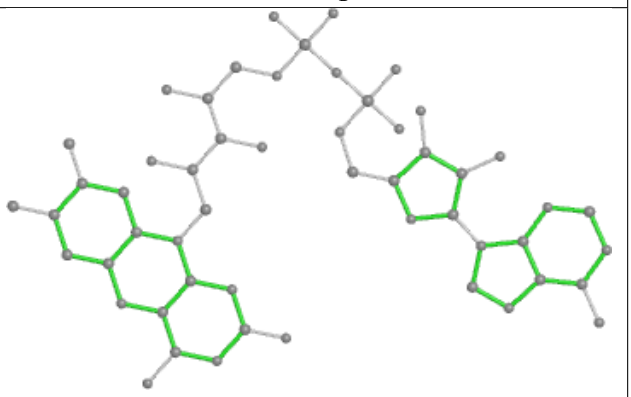
Bond lengths



Bond angles

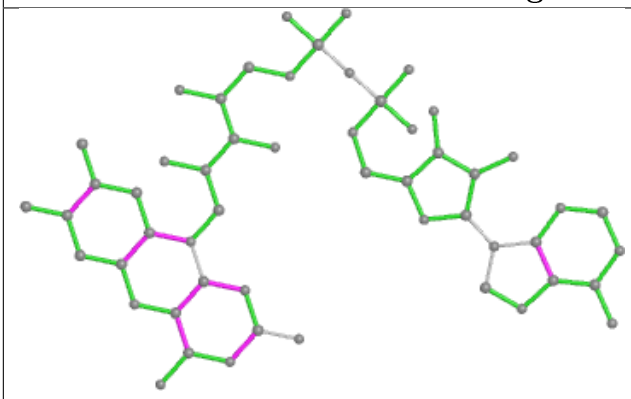


Torsions

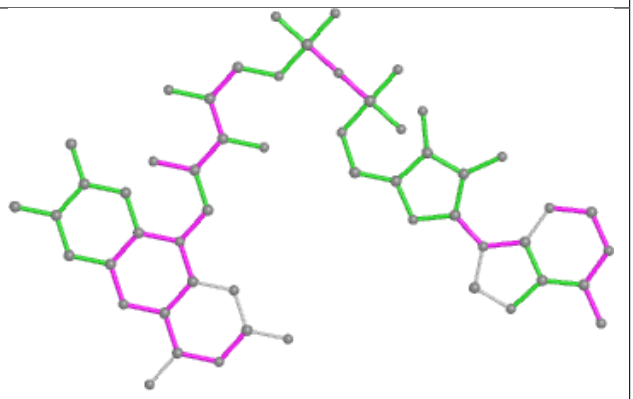


Rings

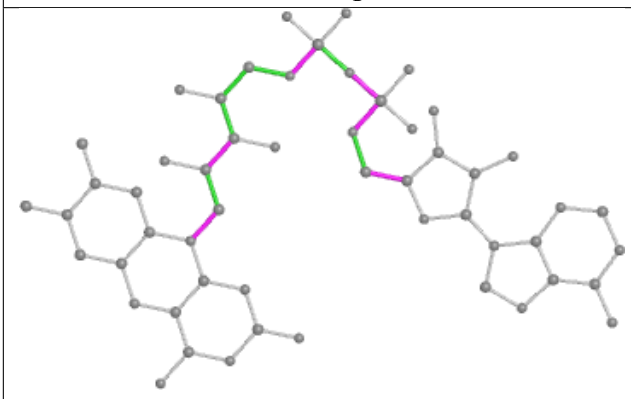
Ligand FAD F 701



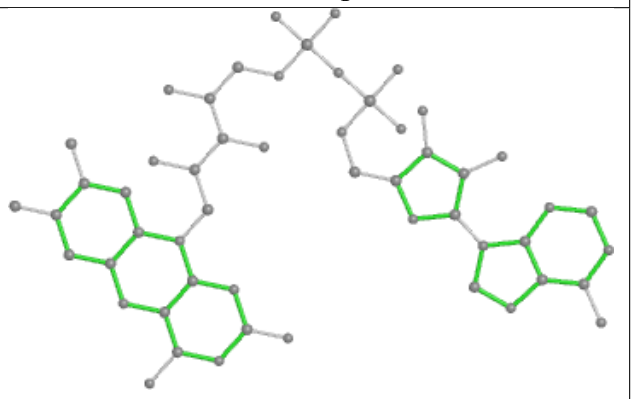
Bond lengths



Bond angles

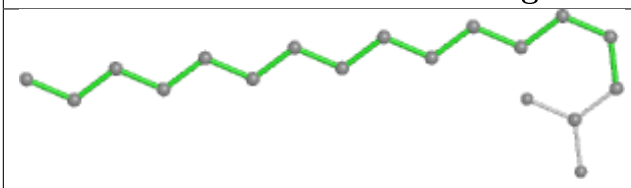


Torsions

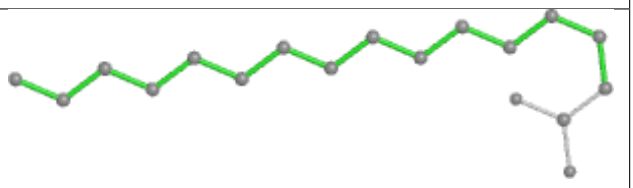


Rings

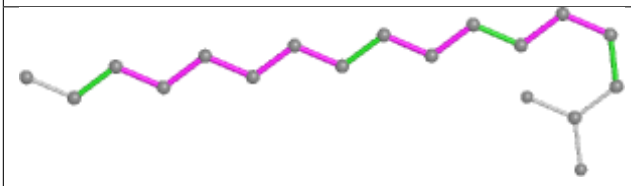
Ligand PLM D 702



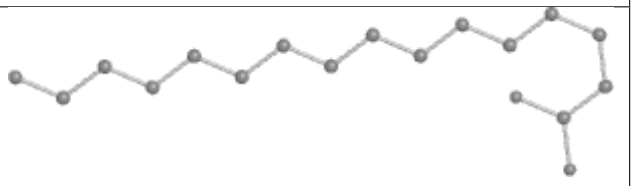
Bond lengths



Bond angles

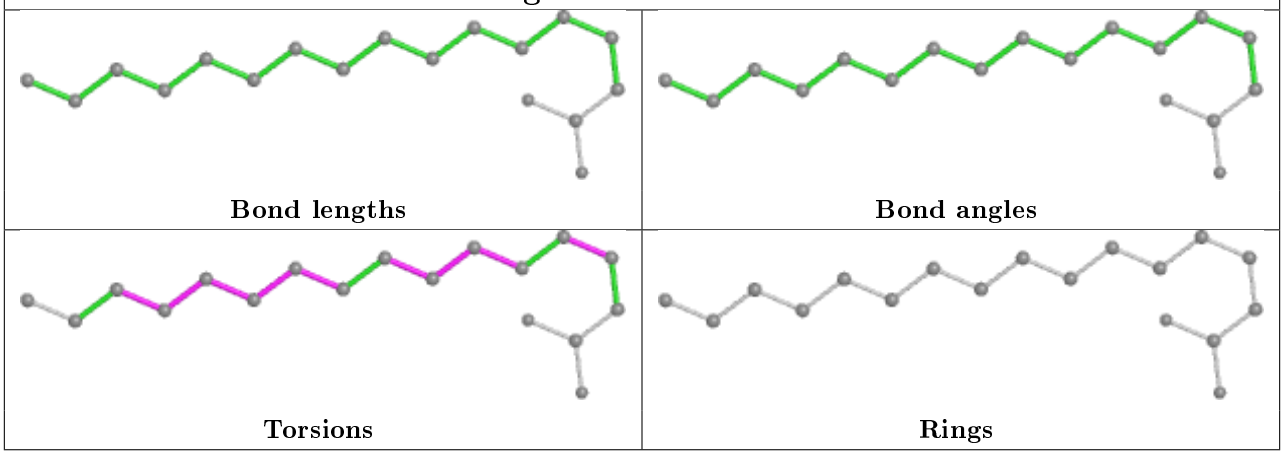


Torsions

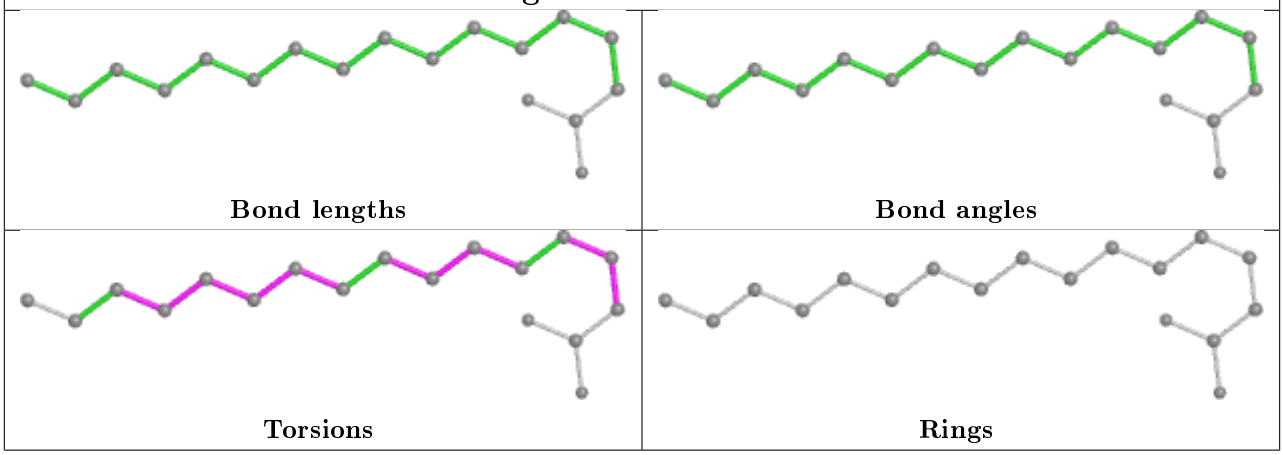


Rings

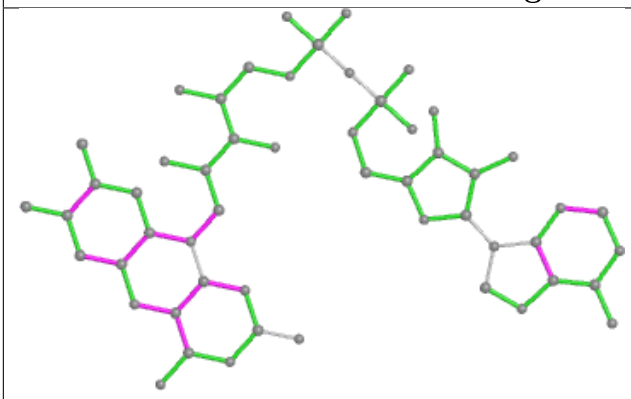
Ligand PLM B 702



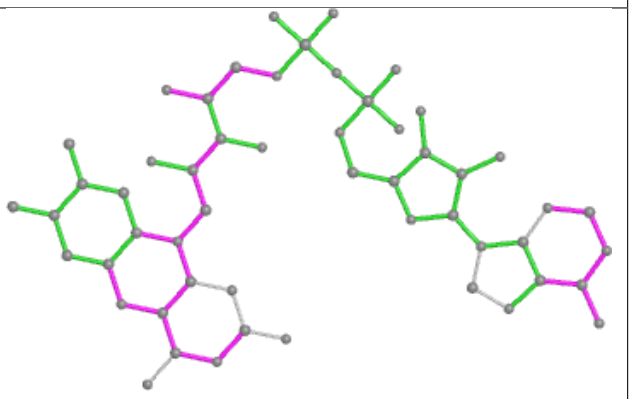
Ligand PLM C 702



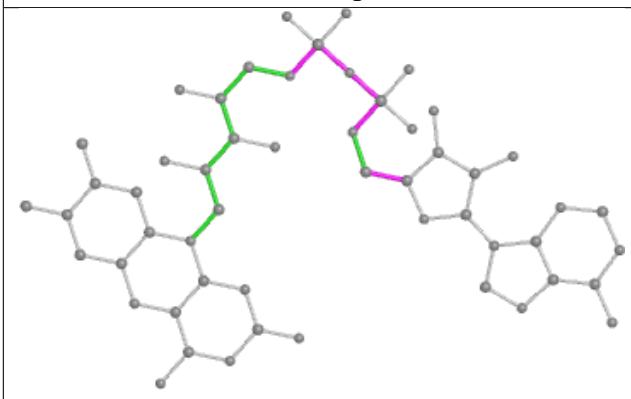
Ligand FAD A 701



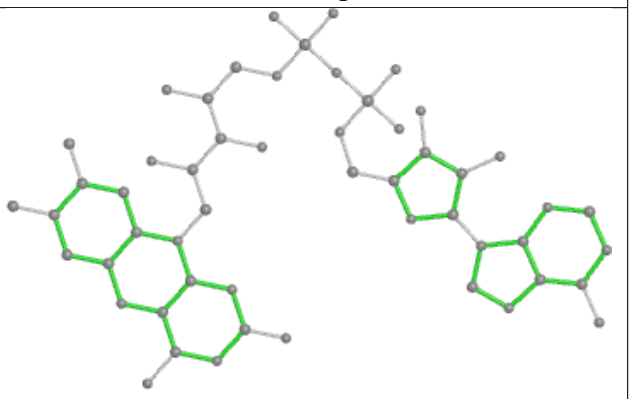
Bond lengths



Bond angles

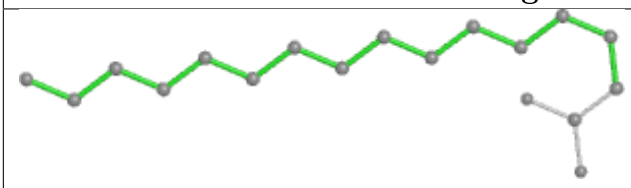


Torsions

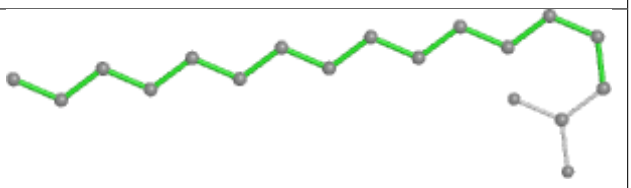


Rings

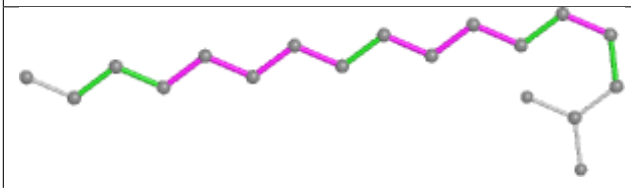
Ligand PLM A 702



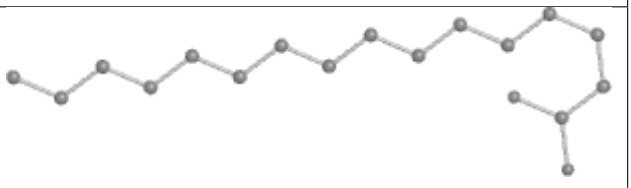
Bond lengths



Bond angles

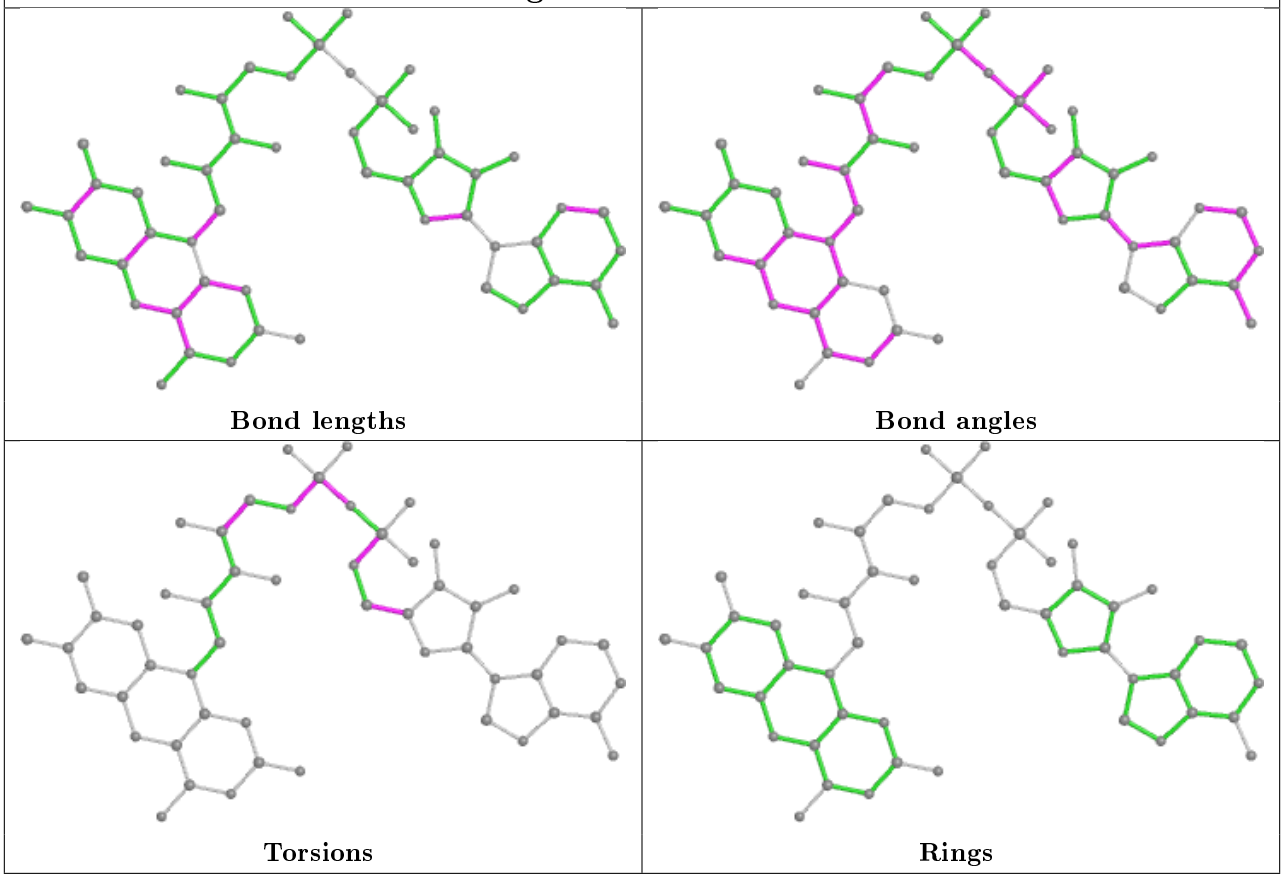


Torsions



Rings

Ligand FAD C 701



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	578/594 (97%)	-0.23	6 (1%) 82 69	20, 41, 75, 102	0
1	B	578/594 (97%)	-0.17	10 (1%) 70 50	21, 43, 77, 119	0
1	C	578/594 (97%)	-0.21	11 (1%) 66 47	22, 44, 79, 114	0
1	D	578/594 (97%)	-0.12	11 (1%) 66 47	24, 48, 78, 132	0
1	E	578/594 (97%)	0.63	61 (10%) 6 2	46, 90, 127, 152	0
1	F	578/594 (97%)	0.51	41 (7%) 16 6	47, 86, 123, 170	0
All	All	3468/3564 (97%)	0.07	140 (4%) 38 19	20, 54, 112, 170	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	419	TYR	6.2
1	E	426	GLY	5.4
1	F	480	PRO	5.4
1	F	229	ASN	5.3
1	E	335	GLY	5.2
1	E	61	SER	4.9
1	F	421	LEU	4.7
1	F	263	THR	4.6
1	F	61	SER	4.6
1	D	68	ILE	4.5
1	E	425	GLY	4.5
1	E	645	SER	4.3
1	C	187	VAL	4.2
1	F	549	GLY	4.2
1	E	334	GLY	4.2
1	F	645	SER	4.2
1	C	308	GLY	4.1
1	E	422	GLY	4.0
1	F	474	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	469	PHE	4.0
1	B	422	GLY	3.9
1	B	229	ASN	3.9
1	B	68	ILE	3.8
1	E	403	HIS	3.8
1	F	68	ILE	3.7
1	D	422	GLY	3.7
1	E	474	SER	3.7
1	C	422	GLY	3.7
1	E	333	PRO	3.7
1	B	474	SER	3.6
1	E	187	VAL	3.6
1	A	421	LEU	3.6
1	E	477	LEU	3.5
1	F	479	TRP	3.5
1	E	68	ILE	3.3
1	C	645	SER	3.3
1	F	644	ALA	3.3
1	F	415	ALA	3.2
1	A	68	ILE	3.2
1	E	100	ASN	3.2
1	F	550	GLU	3.1
1	E	421	LEU	3.1
1	D	421	LEU	3.1
1	F	126	ILE	3.1
1	E	107	SER	3.1
1	C	229	ASN	3.0
1	E	331	LEU	3.0
1	C	68	ILE	3.0
1	E	402	ASP	3.0
1	E	586	ALA	3.0
1	B	421	LEU	3.0
1	B	414	ARG	2.9
1	F	458	LEU	2.9
1	E	479	TRP	2.9
1	D	423	GLY	2.9
1	E	104	ALA	2.9
1	C	396	ASP	2.9
1	E	74	ASP	2.9
1	E	118	ASP	2.8
1	F	226	ARG	2.8
1	F	643	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	187	VAL	2.8
1	E	644	ALA	2.8
1	F	395	TYR	2.8
1	E	188	GLU	2.7
1	E	312	ALA	2.7
1	D	208	PHE	2.7
1	E	355	VAL	2.6
1	D	61	SER	2.6
1	F	476	GLY	2.6
1	F	557	VAL	2.6
1	F	477	LEU	2.5
1	C	550	GLU	2.5
1	E	550	GLU	2.5
1	F	365	GLY	2.5
1	F	426	GLY	2.5
1	C	421	LEU	2.5
1	E	386	LEU	2.5
1	C	69	ARG	2.5
1	E	272	THR	2.5
1	B	188	GLU	2.5
1	E	338	ILE	2.5
1	F	433	ASP	2.5
1	F	552	PHE	2.5
1	D	474	SER	2.5
1	A	550	GLU	2.5
1	A	586	ALA	2.5
1	E	419	TYR	2.5
1	E	281	LEU	2.4
1	F	438	VAL	2.4
1	E	411	ILE	2.4
1	F	235	ALA	2.4
1	F	388	ALA	2.4
1	D	245	LEU	2.4
1	F	429	SER	2.4
1	E	213	TYR	2.4
1	F	538	ALA	2.4
1	E	303	ILE	2.4
1	F	334	GLY	2.4
1	B	550	GLU	2.3
1	E	549	GLY	2.3
1	E	412	ARG	2.3
1	F	430	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	98	LEU	2.3
1	E	75	SER	2.3
1	E	211	GLY	2.3
1	E	336	GLU	2.3
1	E	476	GLY	2.3
1	E	542	ALA	2.3
1	E	600	HIS	2.3
1	B	187	VAL	2.3
1	F	62	ALA	2.3
1	E	101	ARG	2.3
1	E	396	ASP	2.3
1	E	108	LYS	2.3
1	C	188	GLU	2.2
1	E	369	VAL	2.2
1	E	94	ALA	2.2
1	E	212	ALA	2.2
1	F	403	HIS	2.2
1	E	557	VAL	2.2
1	A	70	LYS	2.2
1	D	243	VAL	2.2
1	F	281	LEU	2.2
1	A	62	ALA	2.2
1	D	229	ASN	2.2
1	E	417	ALA	2.1
1	F	274	ALA	2.1
1	F	268	GLN	2.1
1	E	483	ILE	2.1
1	E	293	LEU	2.1
1	E	217	GLY	2.1
1	E	391	VAL	2.0
1	F	131	THR	2.0
1	F	561	ASP	2.0
1	E	62	ALA	2.0
1	F	431	GLY	2.0
1	B	61	SER	2.0
1	E	359	ALA	2.0
1	E	245	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

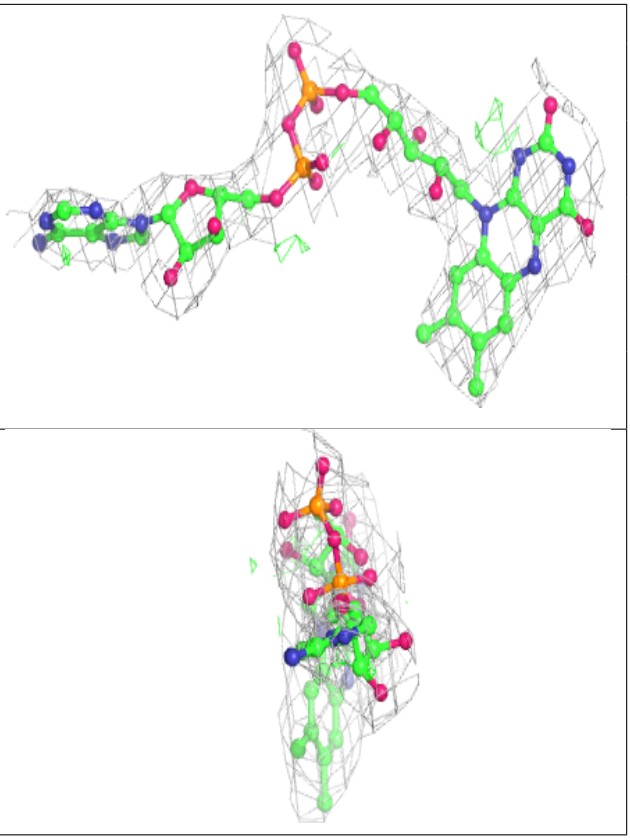
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	E	701	53/53	0.91	0.24	57,85,122,126	0
3	PLM	B	702	18/18	0.91	0.40	31,50,56,58	0
3	PLM	A	702	18/18	0.92	0.25	26,34,43,44	0
2	FAD	F	701	53/53	0.95	0.18	52,65,74,82	0
3	PLM	C	702	18/18	0.95	0.23	29,41,45,45	0
3	PLM	D	702	18/18	0.95	0.24	28,32,35,36	0
2	FAD	D	701	53/53	0.96	0.19	26,33,41,44	0
2	FAD	A	701	53/53	0.96	0.20	26,35,43,44	0
2	FAD	B	701	53/53	0.96	0.20	23,30,42,53	0
2	FAD	C	701	53/53	0.97	0.20	21,32,43,46	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.

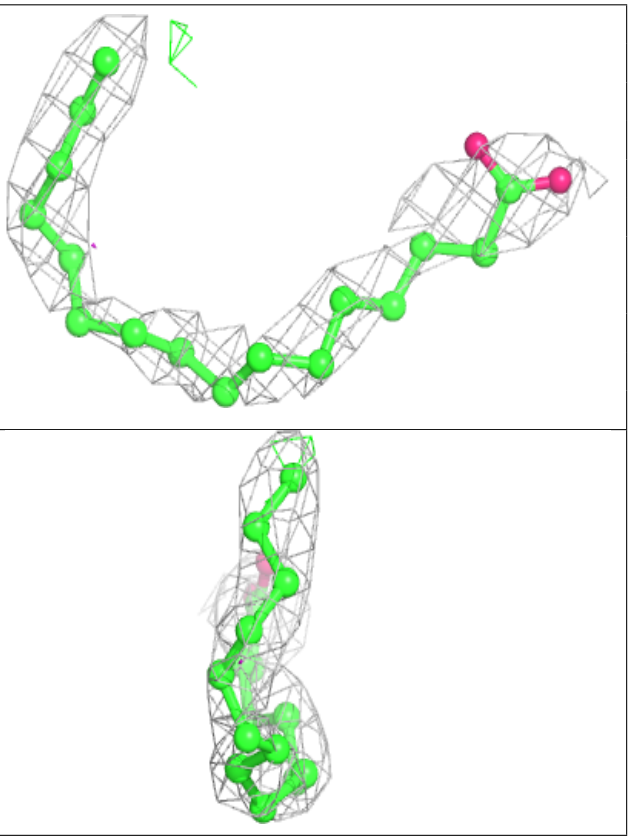
Electron density around FAD E 701:

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



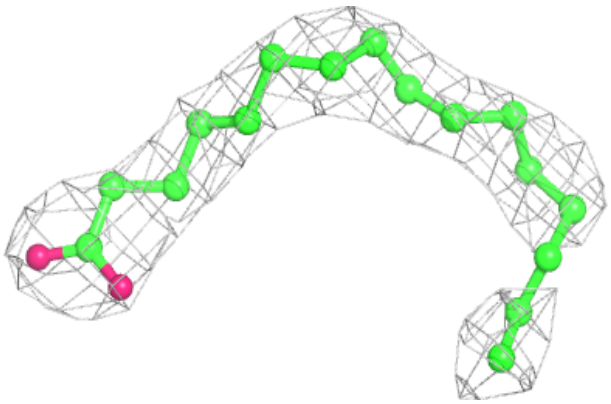
Electron density around PLM B 702:

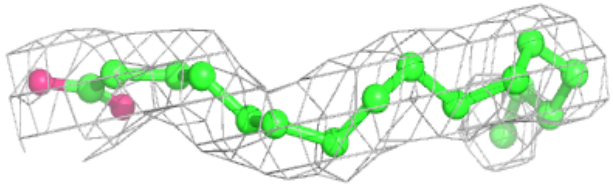
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

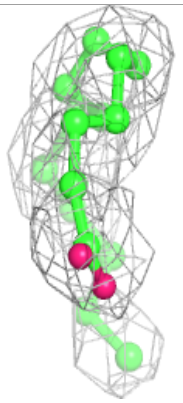


Electron density around PLM A 702:

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

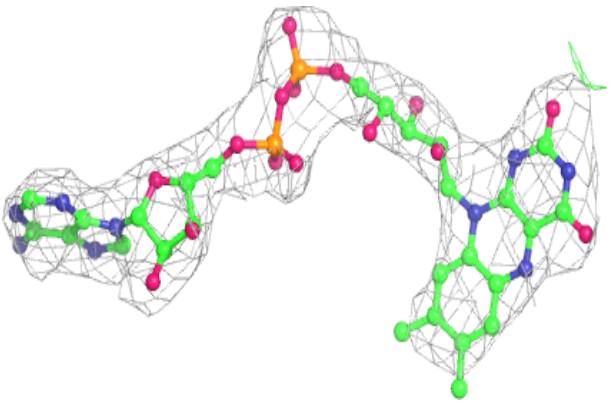


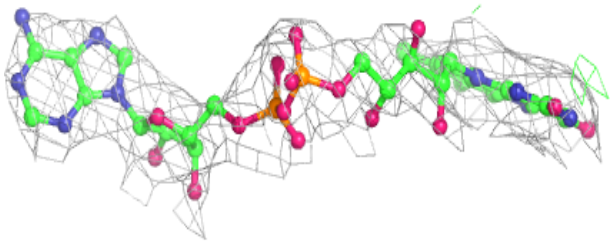


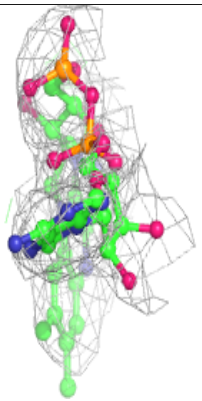


Electron density around FAD F 701:

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

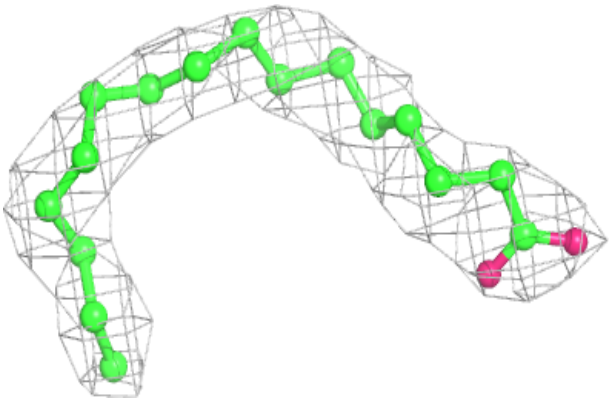


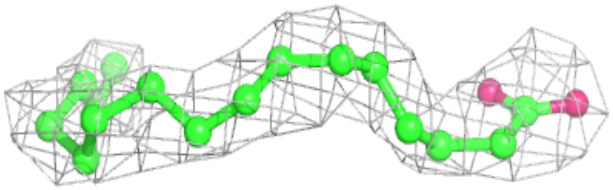


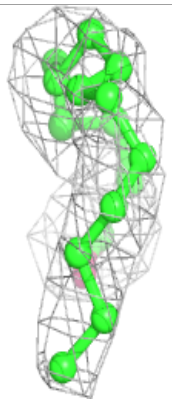


Electron density around PLM C 702:

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

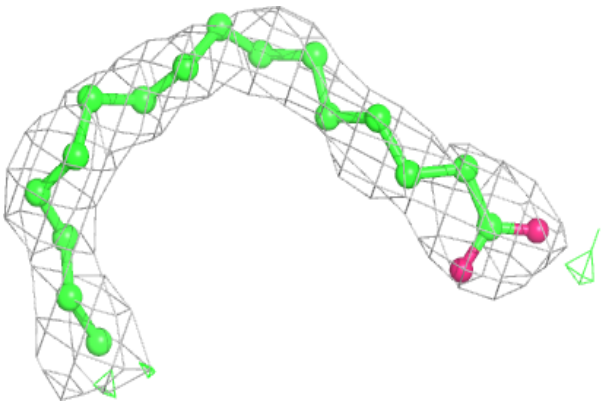


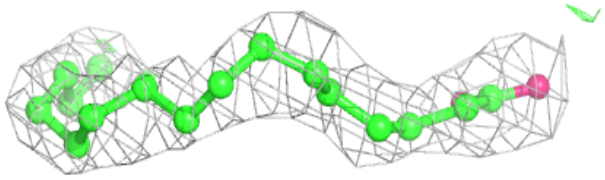


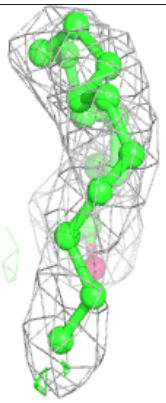


Electron density around PLM D 702:

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

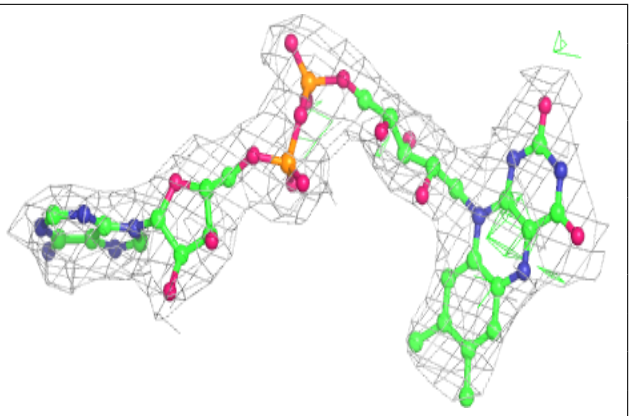


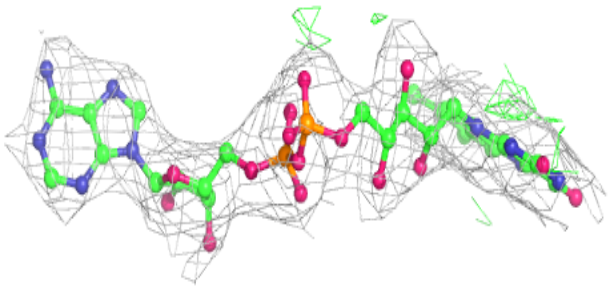


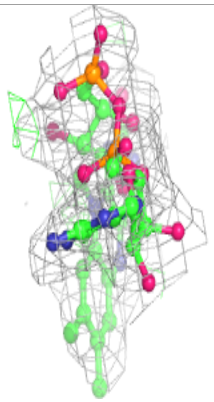


Electron density around FAD D 701:

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

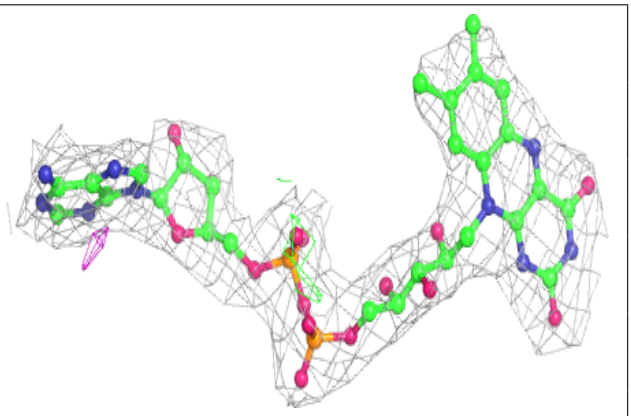


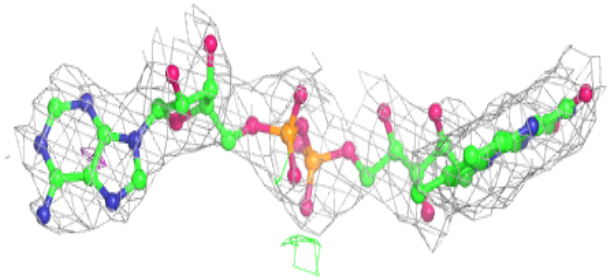




Electron density around FAD A 701:

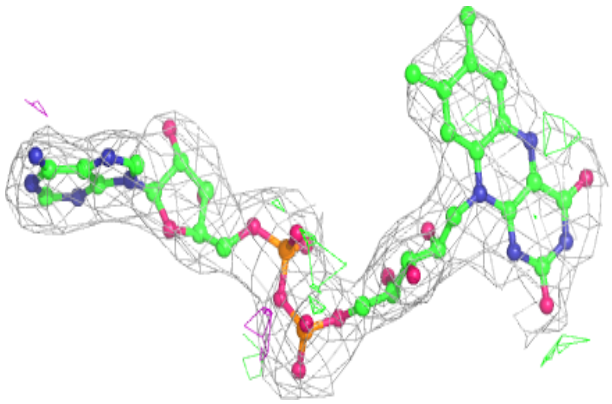
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

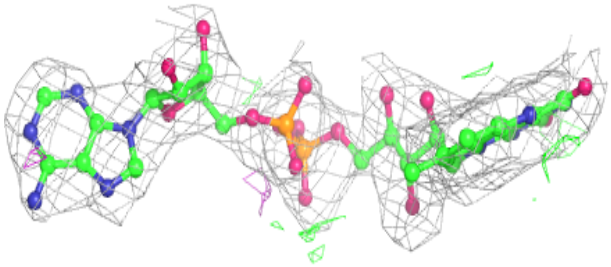


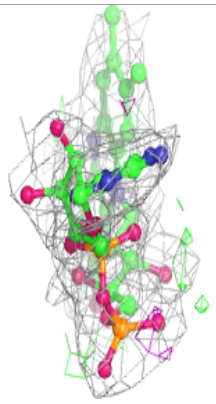


Electron density around FAD B 701:

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

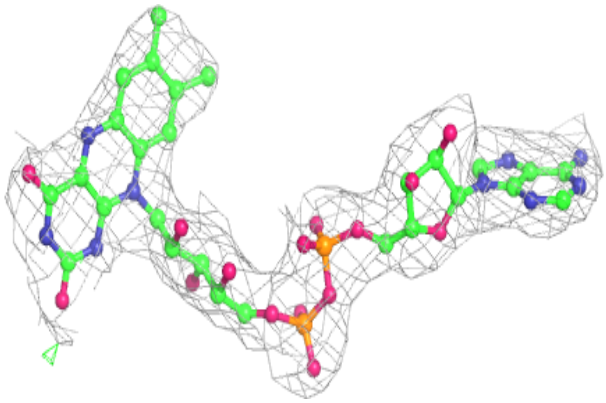


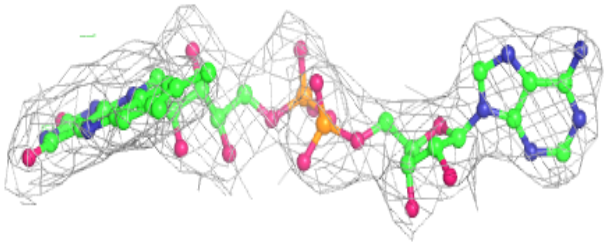


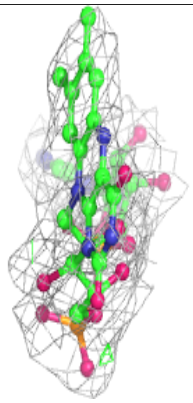


Electron density around FAD C 701:

$2mF_o$-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.