



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:45 AM UTC

PDB ID : 5NCC / pdb_00005ncc
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 types of validation reports are described at

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

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

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

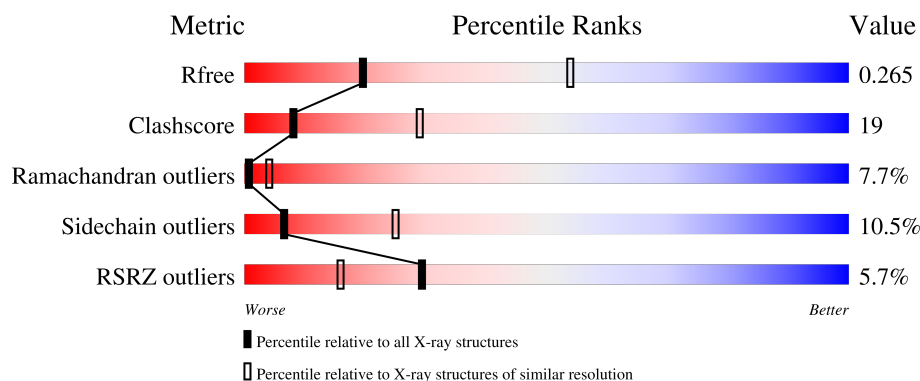
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	594	2% 59% 29% 9% ..
1	B	594	2% 59% 28% 9% ..
1	C	594	3% 59% 27% 9% ..
1	D	594	2% 58% 29% 9% ..
1	E	594	12% 58% 29% 10% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	594	12% 61% 26% 9% ••

2 Entry composition ⓘ

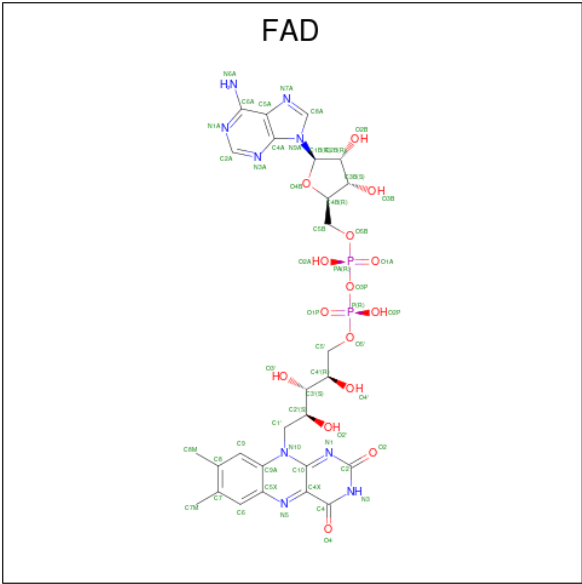
There are 3 unique types of molecules in this entry. The entry contains 26184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

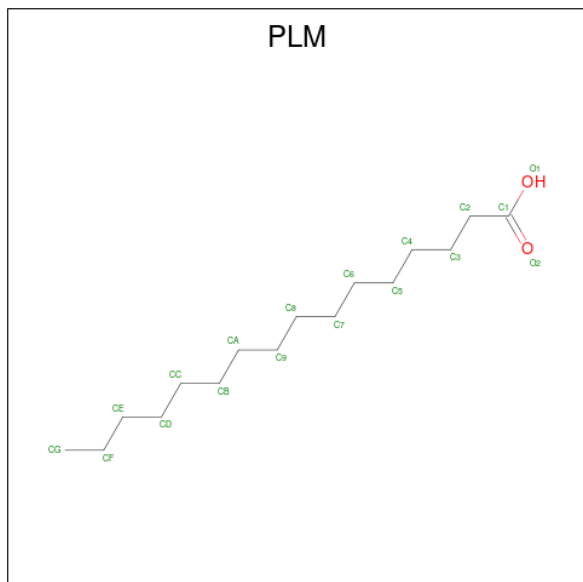
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	B	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	C	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	D	578	Total	C	N	O	S	0	0	0
			4299	2685	769	830	15			
1	E	578	Total	C	N	O	S	0	0	0
			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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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 (CCD ID: PLM) (formula: C₁₆H₃₂O₂).

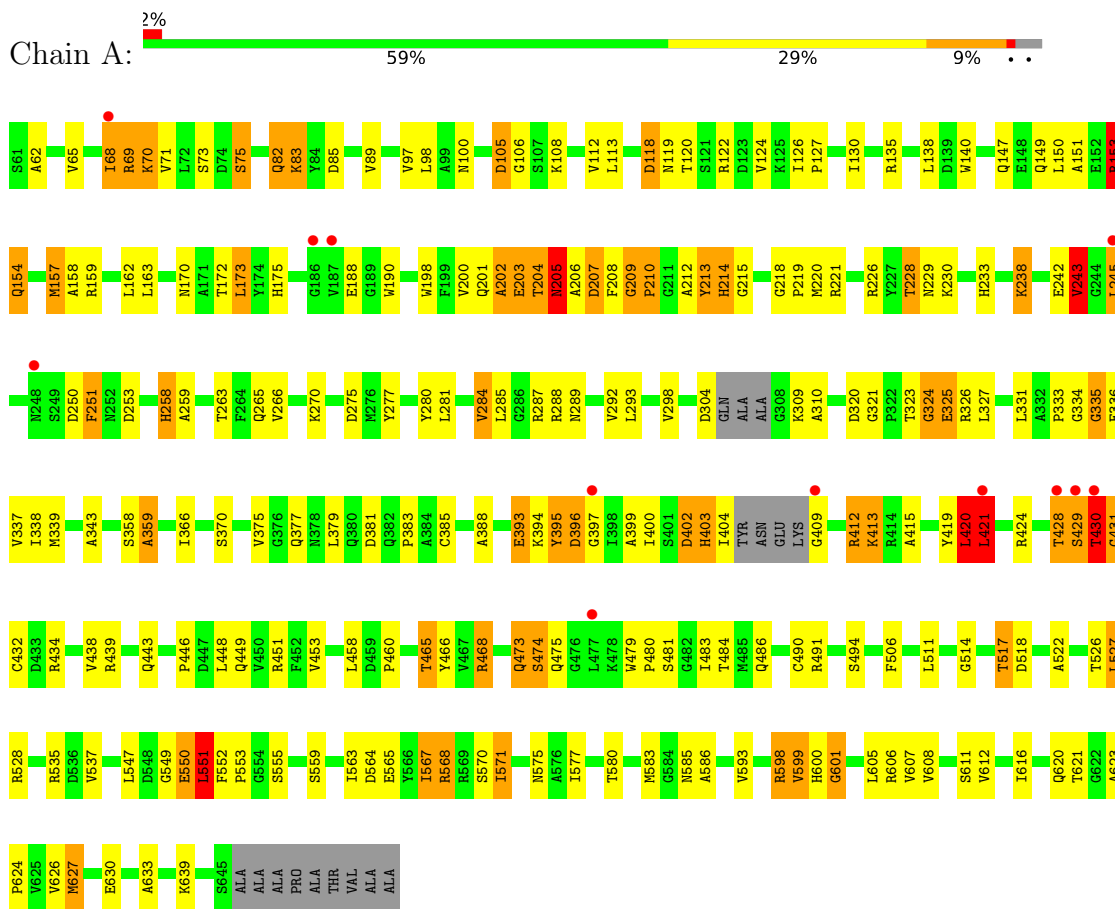


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	16	2		
3	B	1	Total	C	O	0	0
			18	16	2		
3	C	1	Total	C	O	0	0
			18	16	2		
3	D	1	Total	C	O	0	0
			18	16	2		

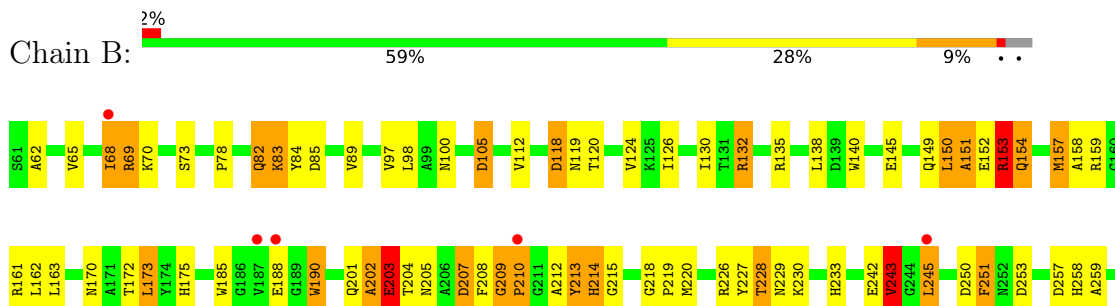
3 Residue-property plots

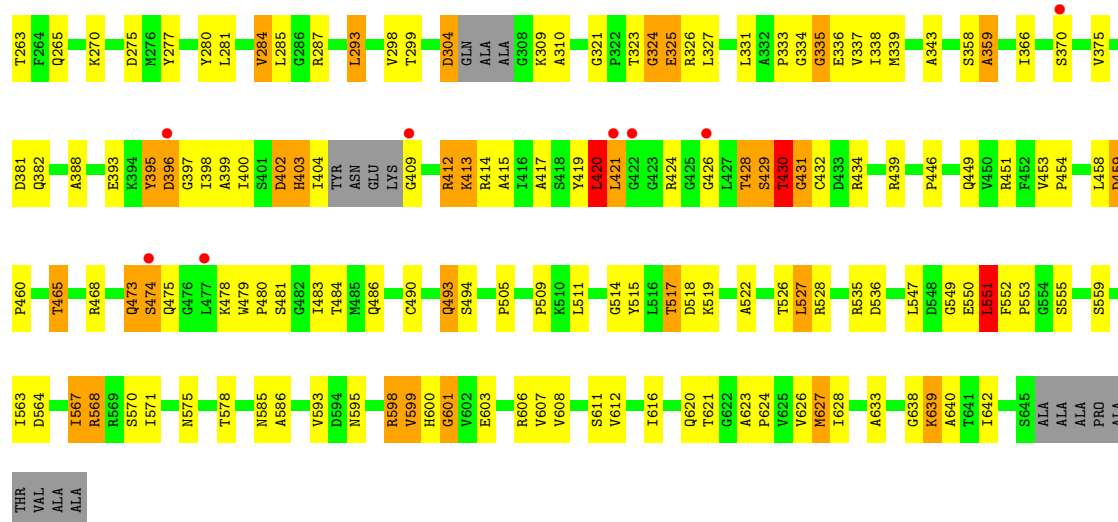
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Fatty acid Photodecarboxylase

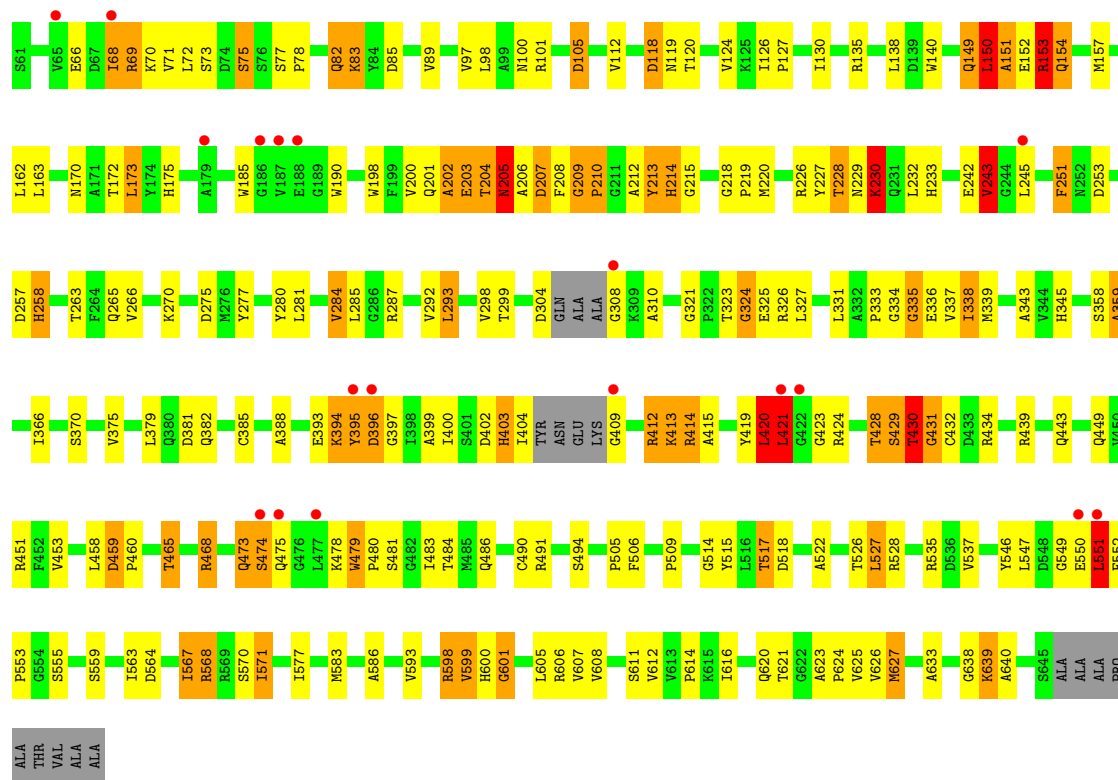


• Molecule 1: Fatty acid Photodecarboxylase



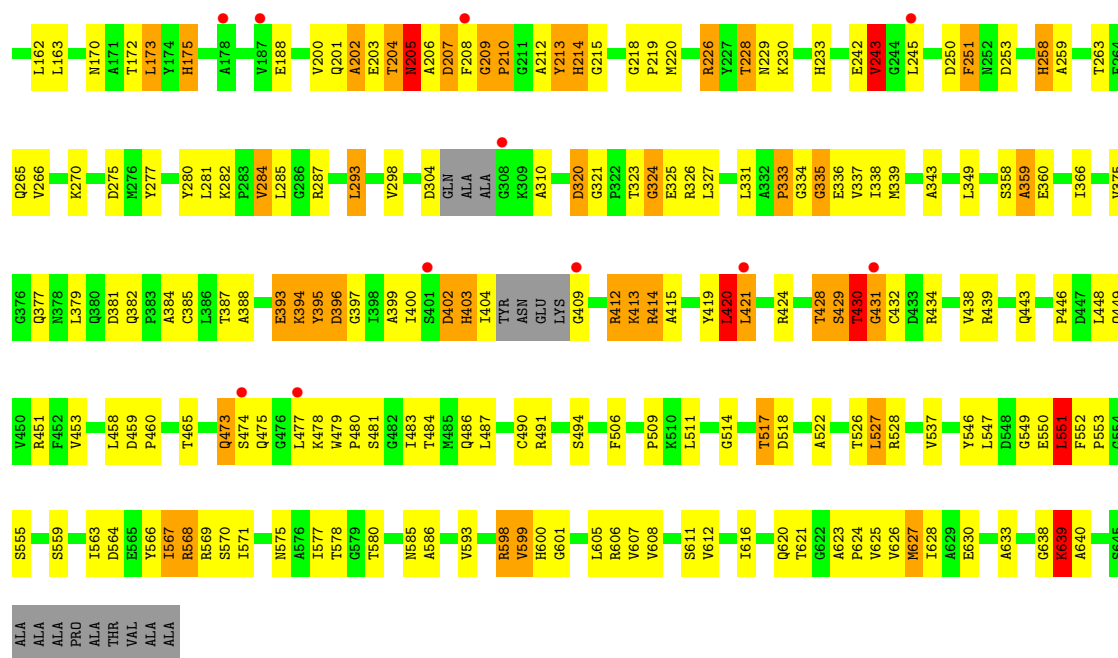


• Molecule 1: Fatty acid Photodecarboxylase

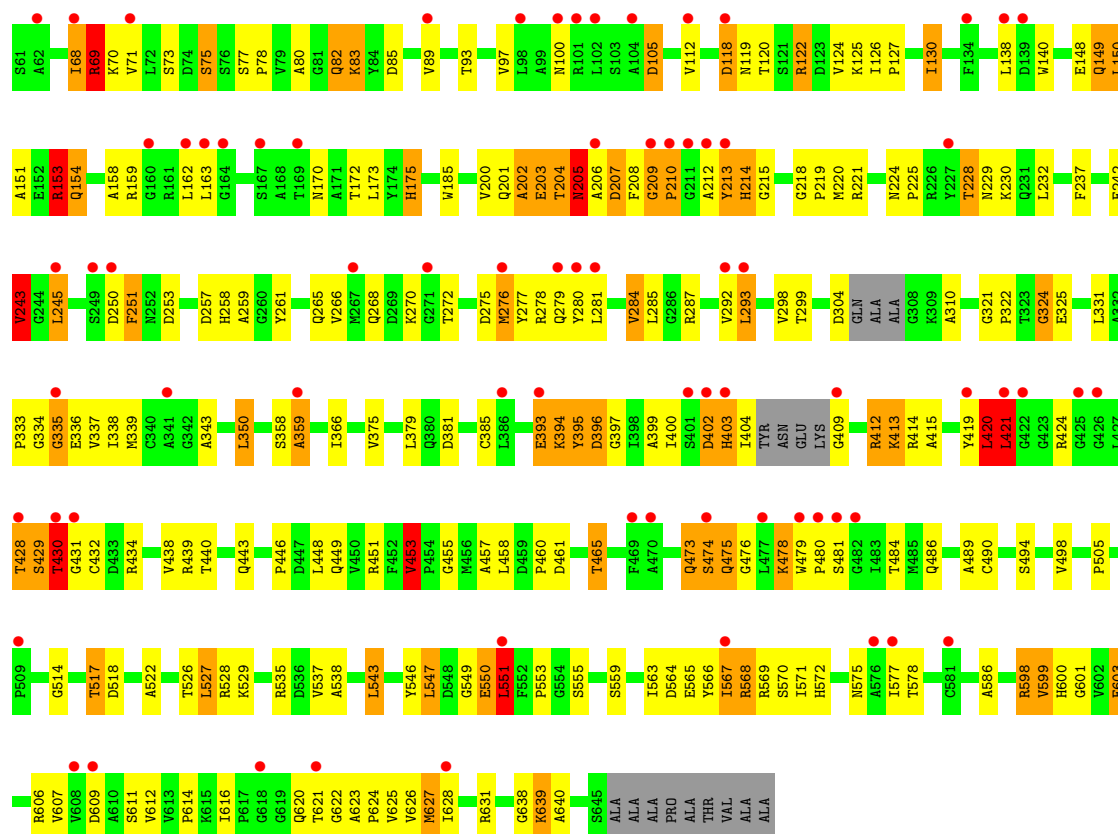


• Molecule 1: Fatty acid Photodecarboxylase





• Molecule 1: Fatty acid Photodecarboxylase



• Molecule 1: Fatty acid Photodecarboxylase



4 Data and refinement statistics

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) 97.3 (49.07-3.12)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (8.30%)	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 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.88	0/4383	1.17	23/5943 (0.4%)
1	B	0.86	0/4383	1.17	23/5943 (0.4%)
1	C	0.87	0/4383	1.18	27/5943 (0.5%)
1	D	0.87	0/4383	1.17	24/5943 (0.4%)
1	E	0.85	1/4383 (0.0%)	1.18	25/5943 (0.4%)
1	F	0.84	0/4383	1.17	24/5943 (0.4%)
All	All	0.86	1/26298 (0.0%)	1.17	146/35658 (0.4%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	631	ARG	C-O	-5.30	1.18	1.24

All (146) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	230	LYS	CA-CB-CG	-10.10	93.89	114.10
1	F	424	ARG	CG-CD-NE	8.09	129.81	112.00
1	A	238	LYS	CB-CG-CD	7.35	128.20	111.30
1	C	82	GLN	CA-C-N	7.34	134.92	121.70
1	C	82	GLN	C-N-CA	7.34	134.92	121.70
1	C	420	LEU	CB-CG-CD2	7.31	132.63	110.70
1	F	82	GLN	CA-C-N	7.21	134.69	121.70
1	F	82	GLN	C-N-CA	7.21	134.69	121.70
1	D	212	ALA	CA-C-N	7.17	134.61	121.70
1	D	212	ALA	C-N-CA	7.17	134.61	121.70
1	C	212	ALA	CA-C-N	7.13	134.53	121.70
1	C	212	ALA	C-N-CA	7.13	134.53	121.70
1	E	82	GLN	CA-C-N	7.12	134.51	121.70
1	E	82	GLN	C-N-CA	7.12	134.51	121.70
1	A	82	GLN	CA-C-N	7.12	134.51	121.70
1	A	82	GLN	C-N-CA	7.12	134.51	121.70
1	F	212	ALA	CA-C-N	7.11	134.49	121.70
1	F	212	ALA	C-N-CA	7.11	134.49	121.70
1	B	212	ALA	CA-C-N	7.10	134.49	121.70
1	B	212	ALA	C-N-CA	7.10	134.49	121.70
1	A	212	ALA	CA-C-N	7.09	134.47	121.70
1	A	212	ALA	C-N-CA	7.09	134.47	121.70
1	E	212	ALA	CA-C-N	7.07	134.43	121.70
1	E	212	ALA	C-N-CA	7.07	134.43	121.70
1	B	82	GLN	CA-C-N	7.07	134.42	121.70
1	B	82	GLN	C-N-CA	7.07	134.42	121.70
1	D	82	GLN	CA-C-N	7.03	134.35	121.70
1	D	82	GLN	C-N-CA	7.03	134.35	121.70
1	F	431	GLY	N-CA-C	-7.01	101.90	112.41
1	A	431	GLY	N-CA-C	-6.85	102.14	112.41
1	F	420	LEU	CA-CB-CG	6.67	139.64	116.30
1	C	431	GLY	N-CA-C	-6.58	102.54	112.41
1	C	150	LEU	CB-CG-CD2	-6.51	91.17	110.70
1	B	431	GLY	N-CA-C	-6.45	102.73	112.41
1	D	139	ASP	CB-CG-OD2	-6.40	103.68	118.40
1	F	126	ILE	CA-CB-CG1	6.35	121.19	110.40
1	D	431	GLY	N-CA-C	-6.34	102.90	112.41
1	E	431	GLY	N-CA-C	-6.32	102.94	112.41
1	A	175	HIS	N-CA-C	6.19	118.49	108.34
1	C	175	HIS	N-CA-C	6.04	118.24	108.34
1	A	221	ARG	CA-CB-CG	6.01	126.12	114.10
1	F	175	HIS	N-CA-C	5.99	118.17	108.34
1	E	421	LEU	CB-CG-CD1	-5.91	92.98	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	335	GLY	N-CA-C	-5.89	104.23	112.13
1	B	509	PRO	N-CA-C	5.82	120.73	114.68
1	F	335	GLY	N-CA-C	-5.71	104.32	112.55
1	F	282	LYS	CB-CG-CD	5.66	124.32	111.30
1	E	547	LEU	CA-CB-CG	5.59	135.87	116.30
1	F	567	ILE	N-CA-C	-5.56	102.35	109.30
1	E	453	VAL	CA-CB-CG1	5.55	119.84	110.40
1	C	321	GLY	CA-C-N	5.52	125.88	119.47
1	C	321	GLY	C-N-CA	5.52	125.88	119.47
1	B	527	LEU	CB-CG-CD1	5.51	127.23	110.70
1	C	335	GLY	N-CA-C	-5.50	104.64	112.55
1	E	479	TRP	CA-C-N	5.49	126.70	119.84
1	E	479	TRP	C-N-CA	5.49	126.70	119.84
1	C	479	TRP	CA-C-N	5.47	126.68	119.84
1	C	479	TRP	C-N-CA	5.47	126.68	119.84
1	B	567	ILE	N-CA-C	-5.47	102.46	109.30
1	D	479	TRP	CA-C-N	5.47	126.68	119.84
1	D	479	TRP	C-N-CA	5.47	126.68	119.84
1	A	567	ILE	N-CA-C	-5.45	102.49	109.30
1	C	567	ILE	N-CA-C	-5.44	102.50	109.30
1	D	567	ILE	N-CA-C	-5.44	102.50	109.30
1	B	490	CYS	CB-CA-C	-5.44	102.27	110.92
1	E	412	ARG	CA-C-N	5.43	131.48	121.70
1	E	412	ARG	C-N-CA	5.43	131.48	121.70
1	A	479	TRP	CA-C-N	5.43	126.62	119.84
1	A	479	TRP	C-N-CA	5.43	126.62	119.84
1	A	335	GLY	N-CA-C	-5.41	104.76	112.55
1	A	153	ARG	CA-C-N	5.39	131.41	121.70
1	A	153	ARG	C-N-CA	5.39	131.41	121.70
1	B	479	TRP	CA-C-N	5.38	126.57	119.84
1	B	479	TRP	C-N-CA	5.38	126.57	119.84
1	B	601	GLY	N-CA-C	5.37	120.58	114.67
1	A	490	CYS	CB-CA-C	-5.36	102.40	110.92
1	B	412	ARG	CA-C-N	5.36	131.34	121.70
1	B	412	ARG	C-N-CA	5.36	131.34	121.70
1	A	412	ARG	CA-C-N	5.35	131.33	121.70
1	A	412	ARG	C-N-CA	5.35	131.33	121.70
1	C	490	CYS	CB-CA-C	-5.34	102.43	110.92
1	E	120	THR	N-CA-C	-5.33	107.43	114.31
1	F	583	MET	CA-CB-CG	5.33	124.77	114.10
1	A	321	GLY	CA-C-N	5.32	125.64	119.47
1	A	321	GLY	C-N-CA	5.32	125.64	119.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	412	ARG	CA-C-N	5.32	131.28	121.70
1	D	412	ARG	C-N-CA	5.32	131.28	121.70
1	B	120	THR	N-CA-C	-5.32	107.45	114.31
1	D	639	LYS	N-CA-C	5.32	122.13	110.80
1	C	120	THR	N-CA-C	-5.30	107.48	114.31
1	F	153	ARG	CA-C-N	5.29	131.22	121.70
1	F	153	ARG	C-N-CA	5.29	131.22	121.70
1	E	335	GLY	N-CA-C	-5.29	104.94	112.55
1	F	509	PRO	N-CA-C	5.28	120.17	114.68
1	F	120	THR	N-CA-C	-5.27	107.51	114.31
1	E	639	LYS	N-CA-C	5.25	121.98	110.80
1	E	153	ARG	CA-C-N	5.24	131.13	121.70
1	E	153	ARG	C-N-CA	5.24	131.13	121.70
1	D	139	ASP	CB-CG-OD1	5.24	130.44	118.40
1	F	321	GLY	CA-C-N	5.22	125.53	119.47
1	F	321	GLY	C-N-CA	5.22	125.53	119.47
1	C	153	ARG	CA-C-N	5.21	131.08	121.70
1	C	153	ARG	C-N-CA	5.21	131.08	121.70
1	C	601	GLY	N-CA-C	5.21	120.40	114.67
1	C	412	ARG	CA-C-N	5.21	131.07	121.70
1	C	412	ARG	C-N-CA	5.21	131.07	121.70
1	F	490	CYS	CB-CA-C	-5.20	102.65	110.92
1	D	321	GLY	CA-C-N	5.20	125.50	119.47
1	D	321	GLY	C-N-CA	5.20	125.50	119.47
1	C	639	LYS	N-CA-C	5.19	121.86	110.80
1	A	601	GLY	N-CA-C	5.19	120.38	114.67
1	D	490	CYS	CB-CA-C	-5.18	102.68	110.92
1	E	212	ALA	N-CA-C	5.17	120.46	114.04
1	D	153	ARG	CA-C-N	5.17	131.01	121.70
1	D	153	ARG	C-N-CA	5.17	131.01	121.70
1	E	321	GLY	CA-C-N	5.16	125.45	119.47
1	E	321	GLY	C-N-CA	5.16	125.45	119.47
1	D	212	ALA	N-CA-C	5.15	120.43	114.04
1	D	120	THR	N-CA-C	-5.15	107.67	114.31
1	A	421	LEU	CA-CB-CG	5.15	134.31	116.30
1	B	321	GLY	CA-C-N	5.14	125.44	119.47
1	B	321	GLY	C-N-CA	5.14	125.44	119.47
1	F	479	TRP	CA-C-N	5.14	126.27	119.84
1	F	479	TRP	C-N-CA	5.14	126.27	119.84
1	B	639	LYS	N-CA-C	5.12	121.71	110.80
1	E	567	ILE	N-CA-C	-5.12	102.90	109.30
1	C	509	PRO	N-CA-C	5.12	120.00	114.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	122	ARG	CB-CG-CD	5.11	123.06	111.30
1	A	120	THR	N-CA-C	-5.11	107.72	114.31
1	D	335	GLY	N-CA-C	-5.10	105.20	112.55
1	F	639	LYS	N-CA-C	5.10	121.66	110.80
1	D	509	PRO	N-CA-C	5.10	119.98	114.68
1	E	490	CYS	CB-CA-C	-5.10	102.81	110.92
1	F	212	ALA	N-CA-C	5.10	120.36	114.04
1	B	212	ALA	N-CA-C	5.09	120.35	114.04
1	D	175	HIS	N-CA-C	5.06	116.64	108.34
1	B	132	ARG	CA-CB-CG	5.04	124.19	114.10
1	D	601	GLY	N-CA-C	5.04	120.21	114.67
1	A	212	ALA	N-CA-C	5.04	120.29	114.04
1	E	601	GLY	N-CA-C	5.04	120.21	114.67
1	C	421	LEU	CA-CB-CG	5.03	133.91	116.30
1	E	175	HIS	N-CA-C	5.03	116.58	108.34
1	C	212	ALA	N-CA-C	5.01	120.25	114.04
1	C	338	ILE	N-CA-C	5.01	115.06	107.75
1	B	153	ARG	CA-C-N	5.00	130.70	121.70
1	B	153	ARG	C-N-CA	5.00	130.70	121.70

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
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

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	175	0
1	B	4299	0	4238	162	1
1	C	4299	0	4238	181	0
1	D	4299	0	4238	177	1
1	E	4299	0	4238	168	0
1	F	4299	0	4238	163	0
2	A	53	0	31	5	0
2	B	53	0	31	5	0
2	C	53	0	31	9	0
2	D	53	0	31	7	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	1010	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 (1010) 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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:LEU:CD2	1:D:421:LEU:HG	1.87	1.03
1:E:429:SER:HB3	1:E:430:THR:HA	1.40	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:D:429:SER:HB3	1:D:430:THR:HA	1.40	1.00
1:E:338:ILE:HG22	1:E:606:ARG:HB2	1.42	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:339:MET:HE2	1:E:350:LEU:HD13	1.62	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
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:459:ASP:CG	1:C:468:ARG:HH21	1.92	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:190:TRP:CD1	1:A:583:MET:HE1	2.23	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:E:598:ARG:O	1:E:599:VAL:HB	1.87	0.72
1:F:400:ILE:CD1	1:F:481:SER:OG	2.36	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:190:TRP:CD1	1:C:583:MET:HE1	2.27	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:97:VAL:HG21	1:F:626:VAL:HG13	1.74	0.68
1:F:226:ARG:HE	1:F:270:LYS:HD3	1.57	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:430:THR:OG1	1:D:431:GLY:N	2.31	0.64
1:E:82:GLN:HA	1:E:83:LYS:HB2	1.79	0.64
1:E:522:ALA:O	1:E:526:THR:HG22	1.98	0.64
1:F:92:GLY:HA3	2:F:701:FAD:O5B	1.98	0.64
1:F:429:SER:CB	1:F:430:THR:CA	2.74	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:82:GLN:HA	1:A:83:LYS:HB2	1.80	0.63
1:A:304:ASP:HB3	1:A:310:ALA:HA	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
1:D:230:LYS:NZ	1:D:397:GLY:HA3	2.12	0.63
1:F:396:ASP:N	1:F:400:ILE:HD13	2.14	0.63
1:F:397:GLY:N	1:F:400:ILE:HB	2.04	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:430:THR:OG1	1:B:431:GLY:N	2.31	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:ALA:HB3	1:B:65:VAL:HG22	1.82	0.60
1:B:228:THR:O	1:B:230:LYS:N	2.34	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:97:VAL:HG21	1:E:626:VAL:HG13	1.83	0.59
1:E:228:THR:O	1:E:230:LYS:N	2.34	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: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
1:D:62:ALA:HB3	1:D:65:VAL:HG22	1.86	0.58
1:D:118:ASP:HB2	1:D:163:LEU:HD12	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:385:CYS:HG	1:A:527:LEU:HD23	1.71	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:E:627:MET:HE3	1:E:628:ILE:HG13	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
1:B:627:MET:HE3	1:B:628:ILE:HG13	1.87	0.55
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:69:ARG:O	1:C:73:SER:HB3	2.05	0.55
1:C:623:ALA:HB3	1:C:624:PRO:HD3	1.89	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:ARG:O	1:D:73:SER:HB3	2.06	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: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:A:220:MET:HE2	1:A:626:VAL:CG1	2.38	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:71:VAL:O	1:C:75:SER:HB3	2.08	0.54
1:C:202:ALA:HA	1:C:218:GLY:HA3	1.89	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:627:MET:HE3	1:D:628:ILE:HG13	1.89	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
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:230:LYS:HZ3	1:E:232:LEU:HD23	1.74	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:TRP:HE1	2:C:701:FAD:H2B	1.73	0.53
1:C:227:TYR:OH	1:C:230:LYS:NZ	2.41	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:339:MET:HB2	1:A:607:VAL:HG12	1.90	0.53
1:A:551:LEU:HB2	1:A:553:PRO:HD2	1.89	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:71:VAL:O	1:F:75:SER:HB3	2.09	0.53
1:F:78:PRO:HG2	1:F:293:LEU:HD21	1.89	0.53
1:A:432:CYS:HB2	1:A:451:ARG:HB3	1.91	0.53
1:B:257:ASP:CG	1:B:439:ARG:HH22	2.16	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:68:ILE:O	1:D:69:ARG:HB3	2.08	0.52
1:D:432:CYS:HB2	1:D:451:ARG:HB3	1.90	0.52
1:E:78:PRO:HG2	1:E:293:LEU:HD21	1.91	0.52
1:E:219:PRO:HG2	1:E:280:TYR:CZ	2.43	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:220:MET:HE2	1:B:626:VAL:CG1	2.40	0.52
1:B:453:VAL:HG21	3:B:702:PLM:H72	1.91	0.52
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:97:VAL:HG21	1:C:626:VAL:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ILE:HG13	1:C:409:GLY:N	2.24	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:71:VAL:O	1:E:75:SER:HB3	2.09	0.52
1:E:130:ILE:HG21	1:E:430:THR:HG21	1.88	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:552:PHE:HA	1:B:68:ILE:HD13	1.93	0.51
1:A:598:ARG:O	1:A:606:ARG:HA	2.11	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
2:B:701:FAD:O2'	2:B:701:FAD:O4'	2.25	0.51
1:C:400:ILE:CD1	1:C:481:SER:CB	2.72	0.51
1:E:230:LYS:HZ1	1:E:397:GLY:HA3	1.76	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
1:D:414:ARG:HE	1:D:414:ARG:HA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:250:ASP:N	1:F:250:ASP:OD2	2.44	0.50
1:F:325:GLU:HG3	1:F:325:GLU:O	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:D:385:CYS:HG	1:D:527:LEU:HD23	1.75	0.50
1:F:105:ASP:OD1	1:F:105:ASP:C	2.54	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:C:190:TRP:CG	1:C:583:MET:HE1	2.47	0.50
1:C:105:ASP:C	1:C:105:ASP:OD1	2.53	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:F:320:ASP:CG	1:F:320:ASP:O	2.55	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:D:230:LYS:HZ1	1:D:397:GLY:HA3	1.77	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD3	1:C:414:ARG:N	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:A:198:TRP:HB2	1:A:627:MET:HE3	1.94	0.49
1:B:220:MET:HE2	1:B:626:VAL:HG11	1.94	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:343:ALA:HA	1:F:611:SER:HB3	1.95	0.49
1:F:460:PRO:HB2	1:F:570:SER:HB2	1.95	0.49
1:C:172:THR:HB	1:C:266:VAL:HG22	1.95	0.49
1:C:220:MET:HE2	1:C:626:VAL:CG1	2.43	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:395:TYR:O	1:B:396:ASP:HB2	2.12	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:251:PHE:C	1:A:253:ASP:H	2.22	0.48
1:B:251:PHE:C	1:B:253:ASP:H	2.22	0.48
1:D:396:ASP:HA	1:D:400:ILE:CG2	2.42	0.48
1:E:77:SER:OG	1:E:80:ALA:CB	2.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:LYS:HE3	1:E:546:TYR:CD1	2.49	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:402:ASP:HA	1:E:412:ARG:HG3	1.95	0.48
1:E:598:ARG:HA	1:E:606:ARG:HG2	1.96	0.48
1:F:212:ALA:C	1:F:213:TYR:HD2	2.21	0.48
1:A:105:ASP:C	1:A:105:ASP:OD1	2.57	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:251:PHE:C	1:C:253:ASP:H	2.22	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:339:MET:HB2	1:D:607:VAL:HG12	1.95	0.48
1:D:395:TYR:O	1:D:396:ASP:HB2	2.13	0.48
1:E:251:PHE:C	1:E:253:ASP:H	2.21	0.48
1:A:220:MET:HE2	1:A:626:VAL:HG11	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:D:251:PHE:C	1:D:253:ASP:H	2.22	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:B:105:ASP:OD1	1:B:105:ASP:C	2.56	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:F:251:PHE:C	1:F:253:ASP:H	2.22	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:A:421:LEU:HD22	1:D:421:LEU:CD1	2.43	0.47
1:B:281:LEU:HG	1:B:285:LEU:HD13	1.96	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:65:VAL:O	1:D:69:ARG:HG2	2.14	0.47
1:D:413:LYS:O	1:D:415:ALA:N	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:324:GLY:O	1:C:325:GLU:HB3	2.13	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
1:D:105:ASP:OD1	1:D:105:ASP:C	2.57	0.47
1:D:324:GLY:O	1:D:325:GLU:HB3	2.14	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:A:157:MET:HE3	1:A:511:LEU:HD22	1.96	0.47
1:A:263:THR:HG23	1:A:434:ARG:HG2	1.96	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:C:395:TYR:O	1:C:396:ASP:HB2	2.13	0.47
1:C:494:SER:HB2	1:C:517:THR:HG22	1.97	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: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:E:105:ASP:C	1:E:105:ASP:OD1	2.57	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:243:VAL:HG11	1:D:537:VAL:HG22	1.97	0.46
1:D:394:LYS:HE3	1:D:546:TYR:CD1	2.51	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
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:B:398:ILE:HG22	1:B:454:PRO:C	2.41	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:400:ILE:HD12	1:B:481:SER:OG	2.13	0.46
1:B:419:TYR:HA	1:B:424:ARG:HA	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:395:TYR:CE1	1:C:478:LYS:NZ	2.73	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:OD1	1:A:381:ASP:O	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:H9	2:C:701:FAD:H1'1	1.73	0.46
1:D:233:HIS:CE1	1:D:434:ARG:HD2	2.50	0.46
1:D:320:ASP:CG	1:D:320:ASP:O	2.59	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: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:77:SER:CB	1:C:327:LEU:HD22	2.46	0.45
1:C:284:VAL:HG13	1:C:287:ARG:HD2	1.97	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:207:ASP:HB3	1:F:265:GLN:HE22	1.81	0.45
1:F:209:GLY:H	1:F:210:PRO:CD	2.26	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:230:LYS:HZ1	1:A:397:GLY:HA3	1.79	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:O	1:F:79:VAL:HG22	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:GLY:O	1:D:640:ALA:N	2.46	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:220:MET:HE2	1:C:626:VAL:HG11	2.00	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:D:549:GLY:C	1:D:551:LEU:H	2.25	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
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:D:220:MET:HE2	1:D:626:VAL:CG1	2.48	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:93:THR:HG23	1:F:276:MET:HG2	1.99	0.44
1:F:414:ARG:HE	1:F:414:ARG:HA	1.82	0.44
1:B:549:GLY:O	1:B:551:LEU:N	2.50	0.44
1:D:220:MET:HE2	1:D:626:VAL:HG11	2.00	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: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:345:HIS:ND1	2:C:701:FAD:H8A	2.33	0.43
1:C:412:ARG:CB	1:C:413:LYS:O	2.61	0.43
1:D:549:GLY:O	1:D:551:LEU:N	2.50	0.43
1:E:324:GLY:O	1:E:325:GLU:HB2	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:GLU:HG2	1:F:215:GLY:O	2.17	0.43
1:A:100:ASN:HA	1:A:284:VAL:HG11	2.00	0.43
1:A:207:ASP:HB3	1:A:265:GLN:HE22	1.82	0.43
1:C:549:GLY:O	1:C:551:LEU:N	2.51	0.43
1:F:480:PRO:O	1:F:481:SER:HB3	2.18	0.43
1:A:113:LEU:HD23	1:A:293:LEU:HD12	2.01	0.43
1:A:280:TYR:OH	1:A:630:GLU:OE2	2.31	0.43
1:A:358:SER:O	1:A:359:ALA:HB3	2.18	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
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:E:535:ARG:HG2	1:E:551:LEU:HD21	2.00	0.43
1:E:549:GLY:C	1:E:551:LEU:H	2.27	0.43
1:A:118:ASP:HA	1:A:163:LEU:HB2	2.00	0.43
1:B:549:GLY:C	1:B:551:LEU:H	2.26	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:A:549:GLY:C	1:A:551:LEU:H	2.26	0.43
1:B:157:MET:HE2	1:B:511:LEU:HD22	2.01	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:H9	2:E:701:FAD:H1'1	1.80	0.43
1:F:393:GLU:CD	1:F:395:TYR:HE2	2.27	0.43
1:A:565:GLU:OE1	1:A:565:GLU:HA	2.18	0.43
1:D:494:SER:HB3	1:D: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:A:494:SER:HB3	1:A:518:ASP:H	1.83	0.43
1:B:417:ALA:HB2	1:C:421:LEU:HA	1.85	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:72:LEU:HD21	1:D:458:LEU:HD22	2.01	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:F:198:TRP:HB2	1:F:627:MET:HE3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:549:GLY:C	1:F:551:LEU:H	2.27	0.43
1:A:243:VAL:HG11	1:A:537:VAL:HG22	2.00	0.43
1:B:190:TRP:CZ3	1:B:595:ASN:O	2.72	0.43
1:B:420:LEU:N	1:B:424:ARG:HD2	2.25	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:A:473:GLN:C	1:A:475:GLN:H	2.27	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
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:243:VAL:CG2	1:B:536:ASP:HB3	2.49	0.42
1:B:451:ARG:HB2	1:B:486:GLN:HB3	2.01	0.42
1:C:358:SER:O	1:C:359:ALA:HB3	2.19	0.42
1:D:528:ARG:HH11	1:D:564:ASP:CG	2.27	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:B:528:ARG:HH11	1:B:564:ASP:CG	2.28	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:270:LYS:O	1:A:424:ARG:HG2	2.19	0.42
1:A:413:LYS:O	1:A:415:ALA:N	2.43	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:C:458:LEU:C	1:C:459:ASP:OD1	2.62	0.42
1:D:172:THR:O	2:D:701:FAD:N3	2.53	0.42
1:D:280:TYR:OH	1:D:630:GLU:OE2	2.27	0.42
1:D:453:VAL:HG21	3:D:702:PLM:C7	2.50	0.42
1:F:528:ARG:HH11	1:F:564:ASP:CG	2.27	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:C:528:ARG:HH11	1:C:564:ASP:CG	2.28	0.42
1:D:387:THR:HA	1:D:553:PRO:HD3	2.01	0.42
1:D:412:ARG:CB	1:D:413:LYS:O	2.61	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:288:ARG:HH12	1:C:66:GLU:HG3	1.85	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: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:F:473:GLN:C	1:F:475:GLN:H	2.28	0.42
1:A:528:ARG:HH11	1:A:564:ASP:CG	2.27	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:473:GLN:C	1:D:475:GLN:H	2.28	0.42
1:D:621:THR:O	1:D:624:PRO:HD2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:358:SER:O	1:E:359:ALA:HB3	2.19	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:549:GLY:C	1:C:551:LEU:H	2.28	0.41
1:C:621:THR:O	1:C:624:PRO:HD2	2.20	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:473:GLN:C	1:E:475:GLN:H	2.28	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:89:VAL:HG13	1:C:298:VAL:HG21	2.01	0.41
1:C:163:LEU:HD23	1:C:163:LEU:HA	1.97	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:E:89:VAL:HG13	1:E:298:VAL:HG21	2.02	0.41
1:E:175:HIS:HB2	1:E:620:GLN:H	1.85	0.41
1:E:343:ALA:HA	1:E:611:SER:HB3	2.01	0.41
1:A:370:SER:CB	1:A:601:GLY:HA3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:ARG:HB2	1:C:633:ALA:HB1	2.02	0.41
1:D:84:TYR:CD2	1:D:111:LEU:HB2	2.56	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: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: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:B:624:PRO:O	1:B:627:MET:HB3	2.20	0.41
1:C:98:LEU:HD23	1:C:633:ALA:HB2	2.02	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:126:ILE:HA	1:E:127:PRO:HD3	1.92	0.41
1:E:335:GLY:HA3	1:E:336:GLU:CB	2.43	0.41
1:E:480:PRO:O	1:E:481:SER:HB3	2.19	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:B:473:GLN:C	1:B:475:GLN:H	2.29	0.40
1:C:473:GLN:C	1:C:475:GLN:H	2.28	0.40
1:D:320:ASP:O	1:D:320:ASP:OD1	2.39	0.40
1:E:528:ARG:HH11	1:E:564:ASP:CG	2.28	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: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:68:ILE:HD13	1:D:552:PHE:HA	2.03	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:HIS:CD2	1:D:620:GLN:HG2	2.53	0.40
1:D:263:THR:HG23	1:D:434:ARG:HG2	2.03	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:C:381:ASP:OD2	1:C:515:TYR:OH	2.31	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

5.3.1 Protein backbone

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	4
1	B	572/594 (96%)	461 (81%)	67 (12%)	44 (8%)	1	4
1	C	572/594 (96%)	464 (81%)	64 (11%)	44 (8%)	1	4
1	D	572/594 (96%)	465 (81%)	63 (11%)	44 (8%)	1	4
1	E	572/594 (96%)	463 (81%)	65 (11%)	44 (8%)	1	4
1	F	572/594 (96%)	466 (82%)	63 (11%)	43 (8%)	1	4
All	All	3432/3564 (96%)	2782 (81%)	387 (11%)	263 (8%)	1	4

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 ⓘ

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%)	401 (90%)	45 (10%)	7	27
1	B	446/455 (98%)	399 (90%)	47 (10%)	6	25
1	C	446/455 (98%)	406 (91%)	40 (9%)	9	31
1	D	446/455 (98%)	399 (90%)	47 (10%)	6	25
1	E	446/455 (98%)	393 (88%)	53 (12%)	5	20
1	F	446/455 (98%)	398 (89%)	48 (11%)	6	23
All	All	2676/2730 (98%)	2396 (90%)	280 (10%)	6	25

All (280) 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	108	LYS
1	A	112	VAL
1	A	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	122	ARG
1	A	130	ILE
1	A	157	MET
1	A	204	THR
1	A	205	ASN
1	A	207	ASP
1	A	213	TYR
1	A	228	THR
1	A	238	LYS
1	A	243	VAL
1	A	245	LEU
1	A	250	ASP
1	A	284	VAL
1	A	309	LYS
1	A	320	ASP
1	A	325	GLU
1	A	366	ILE
1	A	375	VAL
1	A	393	GLU
1	A	394	LYS
1	A	403	HIS
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	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	616	ILE
1	B	85	ASP
1	B	105	ASP
1	B	112	VAL
1	B	118	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	130	ILE
1	B	132	ARG
1	B	150	LEU
1	B	153	ARG
1	B	157	MET
1	B	190	TRP
1	B	203	GLU
1	B	207	ASP
1	B	213	TYR
1	B	228	THR
1	B	243	VAL
1	B	245	LEU
1	B	250	ASP
1	B	284	VAL
1	B	293	LEU
1	B	304	ASP
1	B	309	LYS
1	B	325	GLU
1	B	327	LEU
1	B	366	ILE
1	B	375	VAL
1	B	403	HIS
1	B	414	ARG
1	B	420	LEU
1	B	421	LEU
1	B	428	THR
1	B	429	SER
1	B	430	THR
1	B	459	ASP
1	B	465	THR
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	578	THR
1	B	603	GLU
1	B	612	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	616	ILE
1	C	75	SER
1	C	85	ASP
1	C	105	ASP
1	C	112	VAL
1	C	118	ASP
1	C	130	ILE
1	C	149	GLN
1	C	150	LEU
1	C	157	MET
1	C	204	THR
1	C	205	ASN
1	C	207	ASP
1	C	213	TYR
1	C	228	THR
1	C	230	LYS
1	C	243	VAL
1	C	284	VAL
1	C	293	LEU
1	C	366	ILE
1	C	375	VAL
1	C	394	LYS
1	C	403	HIS
1	C	414	ARG
1	C	420	LEU
1	C	421	LEU
1	C	428	THR
1	C	429	SER
1	C	430	THR
1	C	459	ASP
1	C	465	THR
1	C	468	ARG
1	C	473	GLN
1	C	474	SER
1	C	517	THR
1	C	527	LEU
1	C	551	LEU
1	C	555	SER
1	C	571	ILE
1	C	612	VAL
1	C	616	ILE
1	D	70	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	75	SER
1	D	85	ASP
1	D	105	ASP
1	D	112	VAL
1	D	118	ASP
1	D	130	ILE
1	D	149	GLN
1	D	150	LEU
1	D	153	ARG
1	D	157	MET
1	D	204	THR
1	D	205	ASN
1	D	207	ASP
1	D	213	TYR
1	D	226	ARG
1	D	228	THR
1	D	243	VAL
1	D	250	ASP
1	D	284	VAL
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	428	THR
1	D	429	SER
1	D	430	THR
1	D	459	ASP
1	D	465	THR
1	D	473	GLN
1	D	477	LEU
1	D	517	THR
1	D	527	LEU
1	D	551	LEU
1	D	555	SER
1	D	571	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	578	THR
1	D	612	VAL
1	D	616	ILE
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	130	ILE
1	E	148	GLU
1	E	149	GLN
1	E	150	LEU
1	E	204	THR
1	E	205	ASN
1	E	207	ASP
1	E	213	TYR
1	E	221	ARG
1	E	224	ASN
1	E	228	THR
1	E	243	VAL
1	E	245	LEU
1	E	250	ASP
1	E	276	MET
1	E	284	VAL
1	E	293	LEU
1	E	350	LEU
1	E	366	ILE
1	E	375	VAL
1	E	394	LYS
1	E	403	HIS
1	E	414	ARG
1	E	420	LEU
1	E	421	LEU
1	E	428	THR
1	E	429	SER
1	E	430	THR
1	E	453	VAL
1	E	465	THR
1	E	473	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	474	SER
1	E	475	GLN
1	E	478	LYS
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	571	ILE
1	E	578	THR
1	E	603	GLU
1	E	612	VAL
1	E	616	ILE
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	130	ILE
1	F	150	LEU
1	F	153	ARG
1	F	204	THR
1	F	207	ASP
1	F	213	TYR
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	284	VAL
1	F	293	LEU
1	F	309	LYS
1	F	320	ASP
1	F	327	LEU
1	F	366	ILE
1	F	375	VAL
1	F	394	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	403	HIS
1	F	410	GLN
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
1	F	465	THR
1	F	473	GLN
1	F	517	THR
1	F	527	LEU
1	F	529	LYS
1	F	551	LEU
1	F	571	ILE
1	F	578	THR
1	F	583	MET
1	F	602	VAL
1	F	612	VAL
1	F	616	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	141	ASN
1	A	175	HIS
1	A	224	ASN
1	A	231	GLN
1	A	265	GLN
1	A	289	ASN
1	A	302	ASN
1	A	345	HIS
1	A	352	HIS
1	A	382	GLN
1	A	403	HIS
1	A	475	GLN
1	A	620	GLN
1	B	141	ASN
1	B	147	GLN
1	B	175	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	224	ASN
1	B	258	HIS
1	B	265	GLN
1	B	279	GLN
1	B	345	HIS
1	B	382	GLN
1	B	575	ASN
1	B	585	ASN
1	B	620	GLN
1	C	119	ASN
1	C	175	HIS
1	C	224	ASN
1	C	265	GLN
1	C	279	GLN
1	C	377	GLN
1	C	382	GLN
1	C	585	ASN
1	C	596	GLN
1	C	620	GLN
1	D	175	HIS
1	D	231	GLN
1	D	258	HIS
1	D	265	GLN
1	D	345	HIS
1	D	382	GLN
1	D	486	GLN
1	D	575	ASN
1	D	585	ASN
1	D	620	GLN
1	E	141	ASN
1	E	175	HIS
1	E	224	ASN
1	E	265	GLN
1	E	268	GLN
1	E	279	GLN
1	E	345	HIS
1	E	378	ASN
1	E	380	GLN
1	E	382	GLN
1	E	572	HIS
1	E	585	ASN
1	E	620	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	82	GLN
1	F	141	ASN
1	F	147	GLN
1	F	224	ASN
1	F	258	HIS
1	F	265	GLN
1	F	279	GLN
1	F	291	GLN
1	F	345	HIS
1	F	377	GLN
1	F	382	GLN
1	F	475	GLN
1	F	575	ASN
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 oligosaccharides 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
3	PLM	C	702	-	17,17,17	0.59	0	17,17,17	1.06	1 (5%)
2	FAD	A	701	-	58,58,58	1.70	9 (15%)	85,89,89	1.76	21 (24%)
2	FAD	C	701	-	58,58,58	1.57	11 (18%)	85,89,89	2.02	27 (31%)
2	FAD	B	701	-	58,58,58	1.62	11 (18%)	85,89,89	2.12	26 (30%)
3	PLM	B	702	-	17,17,17	0.75	0	17,17,17	0.77	1 (5%)
2	FAD	E	701	-	58,58,58	1.56	11 (18%)	85,89,89	1.70	16 (18%)
2	FAD	F	701	-	58,58,58	1.66	13 (22%)	85,89,89	1.80	23 (27%)
2	FAD	D	701	-	58,58,58	1.49	9 (15%)	85,89,89	1.96	20 (23%)
3	PLM	D	702	-	17,17,17	0.65	0	17,17,17	0.76	0
3	PLM	A	702	-	17,17,17	0.69	0	17,17,17	0.77	0

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
3	PLM	C	702	-	-	10/15/15/15	-
2	FAD	A	701	-	-	10/34/50/50	0/6/6/6
2	FAD	C	701	-	-	6/34/50/50	0/6/6/6
2	FAD	B	701	-	-	12/34/50/50	0/6/6/6
3	PLM	B	702	-	-	9/15/15/15	-
2	FAD	E	701	-	-	6/34/50/50	0/6/6/6
2	FAD	F	701	-	-	15/34/50/50	0/6/6/6
2	FAD	D	701	-	-	16/34/50/50	0/6/6/6
3	PLM	D	702	-	-	9/15/15/15	-
3	PLM	A	702	-	-	8/15/15/15	-

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	FAD	C9A-C5X	6.09	1.51	1.41
2	A	701	FAD	C5A-C4A	5.77	1.49	1.39
2	F	701	FAD	C9A-C5X	5.57	1.50	1.41
2	E	701	FAD	C9A-C5X	5.43	1.49	1.41
2	B	701	FAD	C9A-C5X	5.30	1.49	1.41
2	E	701	FAD	C5A-C4A	4.90	1.47	1.39
2	C	701	FAD	C9A-C5X	4.85	1.49	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	FAD	C5A-C4A	4.57	1.47	1.39
2	B	701	FAD	C5A-C4A	4.55	1.47	1.39
2	F	701	FAD	C5A-C4A	4.47	1.47	1.39
2	D	701	FAD	C9A-C5X	4.07	1.47	1.41
2	A	701	FAD	C8-C7	4.06	1.50	1.40
2	F	701	FAD	C8-C7	4.01	1.50	1.40
2	B	701	FAD	C8-C7	3.98	1.50	1.40
2	B	701	FAD	C1'-C2'	-3.74	1.47	1.52
2	C	701	FAD	C5A-C4A	3.72	1.45	1.39
2	D	701	FAD	C5A-N7A	-3.59	1.32	1.39
2	C	701	FAD	C8-C7	3.58	1.49	1.40
2	E	701	FAD	C8-C7	3.55	1.49	1.40
2	D	701	FAD	C8-C7	3.35	1.49	1.40
2	E	701	FAD	C5A-C6A	2.88	1.49	1.41
2	C	701	FAD	P-O3P	2.80	1.62	1.59
2	C	701	FAD	C4X-N5	2.79	1.36	1.30
2	E	701	FAD	C4X-N5	2.76	1.36	1.30
2	F	701	FAD	C4-N3	-2.76	1.33	1.38
2	F	701	FAD	PA-O3P	2.74	1.62	1.59
2	F	701	FAD	C10-N10	2.73	1.43	1.37
2	C	701	FAD	C5A-N7A	-2.70	1.34	1.39
2	D	701	FAD	PA-O3P	2.70	1.62	1.59
2	A	701	FAD	C8A-N7A	2.70	1.36	1.31
2	B	701	FAD	P-O3P	2.68	1.62	1.59
2	B	701	FAD	C8A-N7A	2.67	1.36	1.31
2	A	701	FAD	C4-N3	-2.66	1.33	1.38
2	C	701	FAD	C4A-N9A	-2.61	1.32	1.37
2	B	701	FAD	C5X-N5	-2.61	1.34	1.39
2	D	701	FAD	C10-N10	2.61	1.43	1.37
2	A	701	FAD	C4X-N5	2.55	1.36	1.30
2	E	701	FAD	C10-N10	2.53	1.42	1.37
2	C	701	FAD	C4-N3	-2.50	1.34	1.38
2	F	701	FAD	C5A-N7A	-2.49	1.34	1.39
2	A	701	FAD	C5A-N7A	-2.48	1.34	1.39
2	B	701	FAD	C4-N3	-2.48	1.34	1.38
2	F	701	FAD	C5X-N5	-2.44	1.34	1.39
2	C	701	FAD	C8A-N9A	-2.44	1.33	1.37
2	F	701	FAD	C5A-C6A	2.43	1.47	1.41
2	F	701	FAD	C2-N3	-2.36	1.33	1.39
2	D	701	FAD	C4-N3	-2.35	1.34	1.38
2	C	701	FAD	C5A-C6A	2.35	1.47	1.41
2	E	701	FAD	C5A-N7A	-2.34	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	701	FAD	P-O3P	2.34	1.62	1.59
2	F	701	FAD	C4X-N5	2.32	1.35	1.30
2	C	701	FAD	C10-N10	2.30	1.42	1.37
2	E	701	FAD	C8A-N7A	2.28	1.36	1.31
2	E	701	FAD	C4-N3	-2.27	1.34	1.38
2	D	701	FAD	C5X-N5	-2.25	1.35	1.39
2	B	701	FAD	C5A-C6A	2.24	1.47	1.41
2	E	701	FAD	C4X-C10	2.22	1.50	1.44
2	A	701	FAD	C4A-N9A	-2.21	1.33	1.37
2	A	701	FAD	C5A-C6A	2.20	1.47	1.41
2	B	701	FAD	O3'-C3'	2.16	1.48	1.43
2	E	701	FAD	C10-N1	2.13	1.37	1.33
2	F	701	FAD	C4A-N9A	-2.09	1.33	1.37
2	B	701	FAD	C4X-C10	2.08	1.50	1.44
2	D	701	FAD	C5A-C6A	2.03	1.46	1.41

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	FAD	C5A-C4A-N3A	-6.53	117.73	126.72
2	E	701	FAD	C5A-C4A-N3A	-6.25	118.11	126.72
2	B	701	FAD	C4'-C3'-C2'	-6.03	103.54	113.57
2	B	701	FAD	N3A-C4A-N9A	5.92	137.24	127.17
2	D	701	FAD	N3A-C4A-N9A	5.82	137.07	127.17
2	B	701	FAD	C5A-C4A-N3A	-5.77	118.77	126.72
2	C	701	FAD	N3A-C2A-N1A	-5.41	120.39	128.58
2	F	701	FAD	N3A-C4A-N9A	5.08	135.80	127.17
2	F	701	FAD	C5A-C4A-N3A	-5.05	119.76	126.72
2	E	701	FAD	N3A-C4A-N9A	5.02	135.71	127.17
2	A	701	FAD	N3A-C4A-N9A	4.98	135.64	127.17
2	C	701	FAD	N3A-C4A-N9A	4.98	135.64	127.17
2	A	701	FAD	C5A-C4A-N3A	-4.90	119.96	126.72
2	B	701	FAD	C4A-N9A-C8A	4.82	110.80	105.74
2	C	701	FAD	C4A-N9A-C8A	4.82	110.80	105.74
2	C	701	FAD	C5A-C4A-N3A	-4.68	120.27	126.72
2	B	701	FAD	N3A-C2A-N1A	-4.67	121.52	128.58
2	F	701	FAD	C4A-N9A-C8A	4.44	110.40	105.74
2	D	701	FAD	C4'-C3'-C2'	-4.41	106.23	113.57
2	A	701	FAD	O2A-PA-O3P	4.24	118.74	107.27
2	B	701	FAD	C2A-N3A-C4A	4.24	122.19	111.83
2	C	701	FAD	C4-C4X-N5	4.18	123.98	118.21
2	C	701	FAD	C2A-N3A-C4A	4.12	121.90	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	FAD	N3A-C2A-N1A	-4.12	122.34	128.58
2	B	701	FAD	O3'-C3'-C2'	4.01	118.05	108.93
2	D	701	FAD	C2A-N3A-C4A	3.94	121.44	111.83
2	E	701	FAD	C2A-N3A-C4A	3.93	121.42	111.83
2	C	701	FAD	O4B-C1B-N9A	3.88	115.54	108.09
2	A	701	FAD	O3P-PA-O1A	-3.87	99.07	110.70
2	A	701	FAD	N3A-C2A-N1A	-3.82	122.81	128.58
2	E	701	FAD	O4B-C1B-N9A	3.81	115.41	108.09
2	D	701	FAD	N3A-C2A-N1A	-3.73	122.94	128.58
2	D	701	FAD	O3P-PA-O1A	-3.61	99.83	110.70
2	F	701	FAD	C2A-N3A-C4A	3.58	120.58	111.83
2	B	701	FAD	C5'-C4'-C3'	-3.54	105.53	112.22
2	E	701	FAD	C4A-C5A-N7A	-3.40	106.70	110.58
2	D	701	FAD	C4X-C10-N1	-3.39	116.28	124.59
2	A	701	FAD	C2A-N3A-C4A	3.32	119.94	111.83
2	E	701	FAD	N3A-C2A-N1A	-3.31	123.58	128.58
2	D	701	FAD	O4B-C1B-N9A	3.24	114.30	108.09
2	C	701	FAD	C9A-C5X-N5	-3.17	119.09	122.45
2	B	701	FAD	N9A-C8A-N7A	-3.17	109.44	113.94
2	A	701	FAD	C4-C4X-N5	3.15	122.56	118.21
2	E	701	FAD	C5X-C9A-N10	3.14	120.81	117.97
2	C	701	FAD	O3P-PA-O1A	-3.14	101.27	110.70
2	F	701	FAD	C4X-C10-N1	-3.11	116.96	124.59
2	A	701	FAD	N6A-C6A-N1A	3.06	125.19	118.38
2	D	701	FAD	O2A-PA-O3P	3.02	115.45	107.27
2	C	701	FAD	C10-N1-C2	3.01	123.37	116.85
2	B	701	FAD	C5X-C9A-N10	2.99	120.67	117.97
2	A	701	FAD	O2P-P-O3P	2.97	115.30	107.27
2	A	701	FAD	C4A-N9A-C8A	2.95	108.83	105.74
2	A	701	FAD	O3P-P-O1P	-2.94	101.85	110.70
2	D	701	FAD	N6A-C6A-N1A	2.92	124.88	118.38
2	C	701	FAD	C5X-N5-C4X	2.89	122.75	118.09
2	B	701	FAD	O4'-C4'-C5'	2.86	116.29	109.99
2	A	701	FAD	C10-N1-C2	2.81	122.92	116.85
2	D	701	FAD	C10-N1-C2	2.80	122.90	116.85
2	C	701	FAD	C4X-C10-N1	-2.78	117.78	124.59
2	B	701	FAD	C5A-C6A-N6A	-2.77	116.43	123.29
2	D	701	FAD	O2P-P-O3P	2.76	114.73	107.27
2	C	701	FAD	O2A-PA-O1A	2.74	125.21	112.44
2	F	701	FAD	N9A-C8A-N7A	-2.74	110.05	113.94
2	B	701	FAD	O3P-PA-O1A	-2.72	102.51	110.70
2	F	701	FAD	C5'-C4'-C3'	-2.69	107.14	112.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	701	FAD	O2A-PA-O1A	2.69	124.97	112.44
2	C	701	FAD	N9A-C8A-N7A	-2.68	110.14	113.94
2	B	701	FAD	O2P-P-O1P	2.67	124.88	112.44
2	B	701	FAD	O3P-P-O1P	-2.66	102.70	110.70
2	C	701	FAD	C5'-C4'-C3'	-2.66	107.21	112.22
2	F	701	FAD	C10-N1-C2	2.64	122.57	116.85
2	D	701	FAD	O3'-C3'-C2'	2.64	114.94	108.93
2	B	701	FAD	C5A-N7A-C8A	2.64	107.60	103.45
2	B	701	FAD	O2A-PA-O1A	2.64	124.72	112.44
2	E	701	FAD	O4-C4-C4X	-2.64	119.57	126.53
2	D	701	FAD	C5'-C4'-C3'	-2.63	107.26	112.22
3	C	702	PLM	C3-C2-C1	-2.63	107.66	114.51
2	F	701	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	A	701	FAD	O4'-C4'-C5'	-2.60	104.25	109.99
2	F	701	FAD	C5A-N7A-C8A	2.58	107.51	103.45
2	D	701	FAD	C5A-C6A-N6A	-2.58	116.90	123.29
2	C	701	FAD	C4B-O4B-C1B	-2.58	103.78	109.47
2	E	701	FAD	C5A-N7A-C8A	2.53	107.43	103.45
2	C	701	FAD	C4'-C3'-C2'	-2.53	109.37	113.57
2	A	701	FAD	C5A-C6A-N6A	-2.52	117.04	123.29
2	B	701	FAD	N6A-C6A-N1A	2.51	123.98	118.38
2	E	701	FAD	C4X-C10-N1	-2.50	118.47	124.59
2	F	701	FAD	C4X-C4-N3	2.48	119.57	113.25
2	C	701	FAD	C2A-N1A-C6A	2.48	122.80	118.73
2	F	701	FAD	O2A-PA-O3P	2.47	113.96	107.27
2	F	701	FAD	O2'-C2'-C3'	2.47	115.03	109.25
2	A	701	FAD	C2A-N1A-C6A	2.47	122.78	118.73
2	A	701	FAD	O4-C4-C4X	-2.45	120.08	126.53
2	D	701	FAD	O2'-C2'-C3'	-2.44	103.54	109.25
2	B	701	FAD	C8M-C8-C9	-2.40	115.34	119.57
2	F	701	FAD	C2A-N1A-C6A	2.39	122.66	118.73
2	B	701	FAD	O2P-P-O3P	2.36	113.67	107.27
2	D	701	FAD	C4X-C10-N10	2.36	119.86	116.48
2	C	701	FAD	C10-C4X-N5	-2.35	120.00	124.81
2	E	701	FAD	C4A-N9A-C8A	2.35	108.21	105.74
2	A	701	FAD	C4X-C4-N3	2.35	119.24	113.25
2	B	701	FAD	O2-C2-N1	-2.33	117.93	121.80
2	D	701	FAD	C2B-C1B-N9A	-2.33	107.52	113.30
2	A	701	FAD	C1'-C2'-C3'	-2.32	103.38	109.66
2	C	701	FAD	N6A-C6A-N1A	2.30	123.51	118.38
2	D	701	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	A	701	FAD	C4X-C10-N1	-2.29	118.98	124.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	701	FAD	N10-C10-N1	2.28	125.22	118.51
2	C	701	FAD	C4A-C5A-N7A	-2.25	108.02	110.58
2	C	701	FAD	C5A-N7A-C8A	2.24	106.97	103.45
2	E	701	FAD	C4X-C4-N3	2.24	118.95	113.25
2	A	701	FAD	O5'-C5'-C4'	-2.23	103.41	109.36
2	F	701	FAD	C2'-C1'-N10	2.22	120.72	110.20
2	E	701	FAD	C9A-C5X-N5	-2.22	120.10	122.45
2	C	701	FAD	C4X-C4-N3	2.20	118.86	113.25
2	B	701	FAD	C9A-C5X-N5	-2.18	120.14	122.45
2	C	701	FAD	O4B-C4B-C3B	2.18	109.48	105.15
2	C	701	FAD	C5A-C6A-N6A	-2.17	117.92	123.29
2	A	701	FAD	C7M-C7-C6	-2.16	115.78	119.57
2	F	701	FAD	O3P-PA-O1A	-2.15	104.22	110.70
2	B	701	FAD	C4A-C5A-N7A	-2.14	108.14	110.58
2	E	701	FAD	C6A-C5A-N7A	2.14	136.21	132.09
2	B	701	FAD	C1'-N10-C9A	-2.11	116.53	120.63
2	F	701	FAD	C4-C4X-N5	2.08	121.09	118.21
2	C	701	FAD	O3P-P-O1P	-2.08	104.45	110.70
2	F	701	FAD	C5X-C9A-N10	2.07	119.84	117.97
2	F	701	FAD	C9A-C5X-N5	-2.05	120.28	122.45
2	F	701	FAD	O4-C4-C4X	-2.05	121.12	126.53
2	F	701	FAD	N6A-C6A-N1A	2.05	122.94	118.38
2	D	701	FAD	O3P-P-O1P	-2.03	104.59	110.70
2	E	701	FAD	O3P-PA-O1A	-2.03	104.59	110.70
2	B	701	FAD	O5'-P-O1P	-2.03	100.90	108.94
3	B	702	PLM	C3-C2-C1	-2.02	109.25	114.51
2	C	701	FAD	C6-C5X-N5	2.01	121.78	118.44
2	B	701	FAD	C4X-C10-N1	-2.01	119.67	124.59

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	FAD	C5'-O5'-P-O2P
2	B	701	FAD	C5B-O5B-PA-O1A
2	B	701	FAD	C5B-O5B-PA-O2A
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	C5'-O5'-P-O3P
2	B	701	FAD	PA-O3P-P-O5'
2	C	701	FAD	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

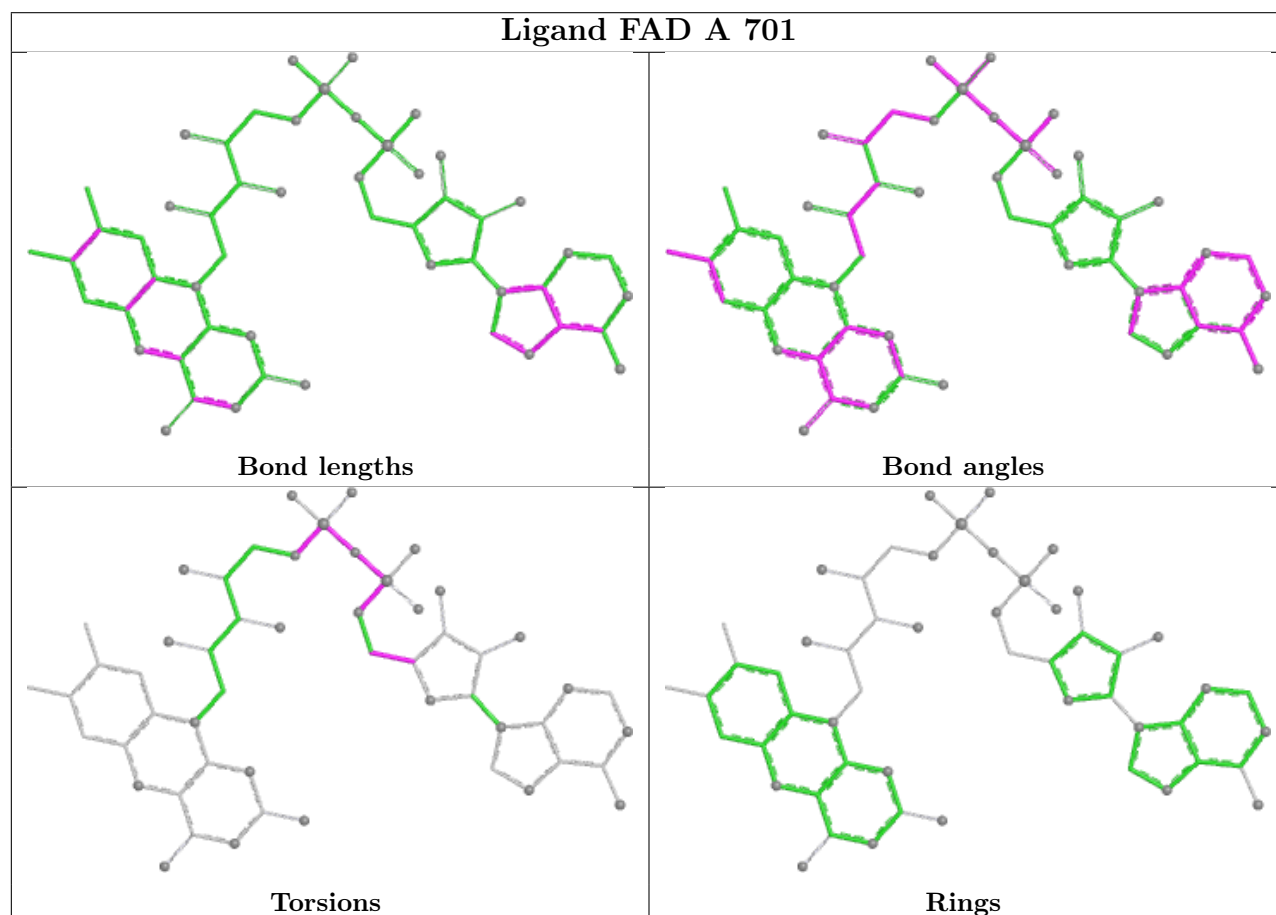
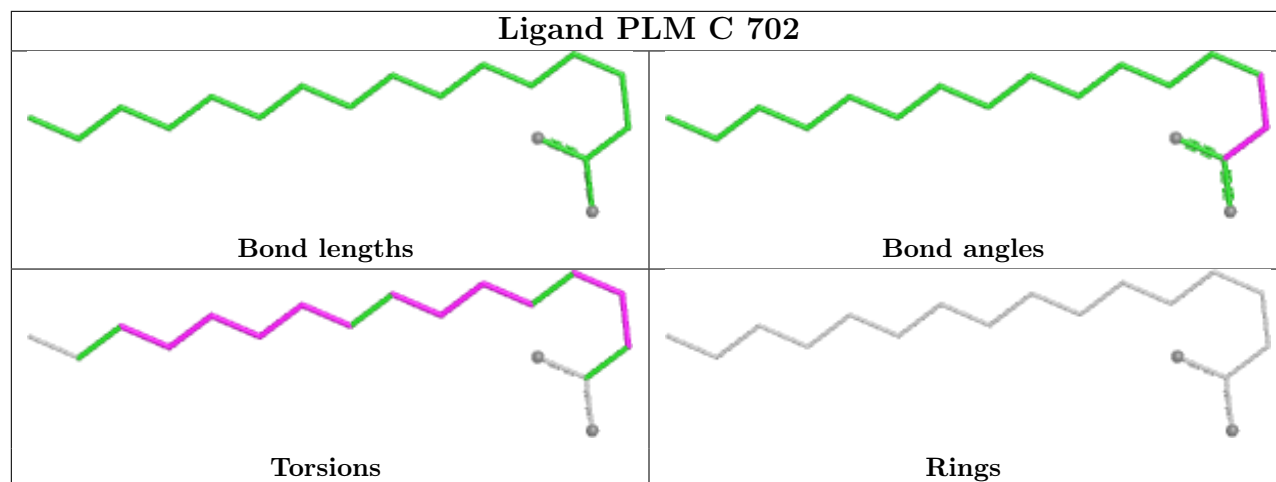
Mol	Chain	Res	Type	Atoms
3	D	702	PLM	C3-C4-C5-C6
2	D	701	FAD	PA-O3P-P-O1P
2	F	701	FAD	P-O3P-PA-O1A
2	F	701	FAD	P-O3P-PA-O2A
3	B	702	PLM	CC-CD-CE-CF
3	C	702	PLM	C8-C9-CA-CB
3	C	702	PLM	C9-CA-CB-CC
2	D	701	FAD	P-O3P-PA-O2A

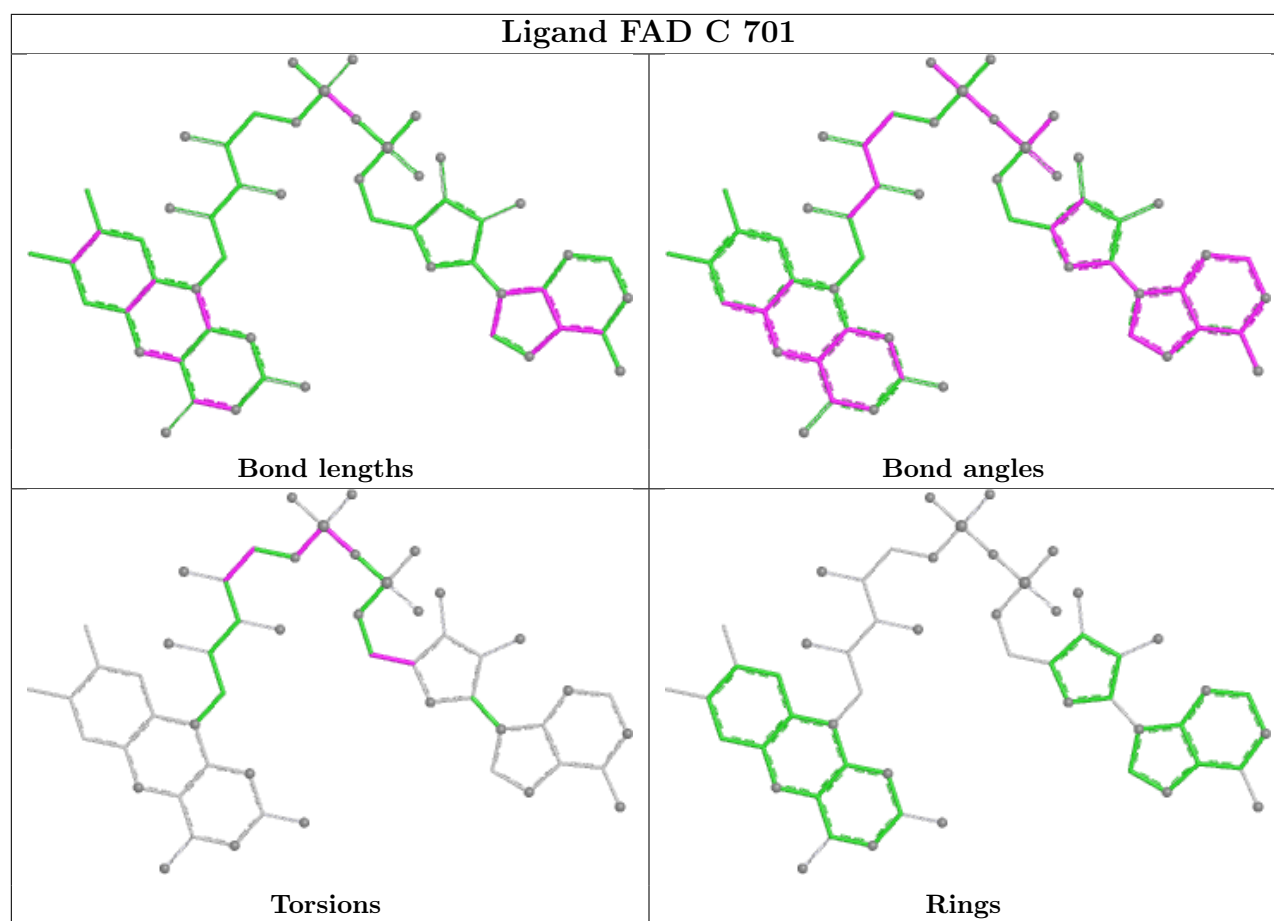
There are no ring outliers.

10 monomers are involved in 55 short contacts:

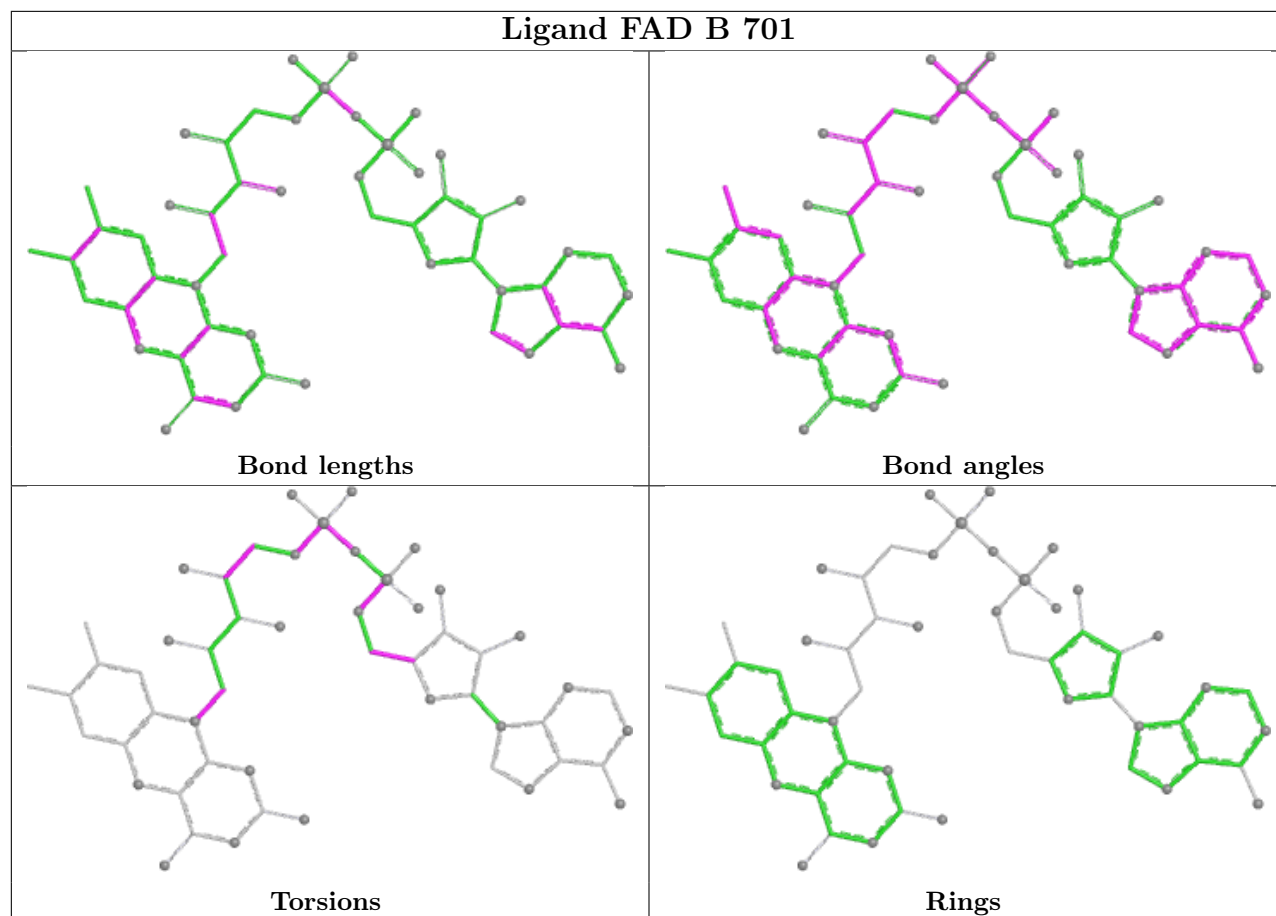
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	PLM	3	0
2	A	701	FAD	5	0
2	C	701	FAD	9	0
2	B	701	FAD	5	0
3	B	702	PLM	4	0
2	E	701	FAD	7	0
2	F	701	FAD	5	0
2	D	701	FAD	7	0
3	D	702	PLM	3	0
3	A	702	PLM	7	0

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

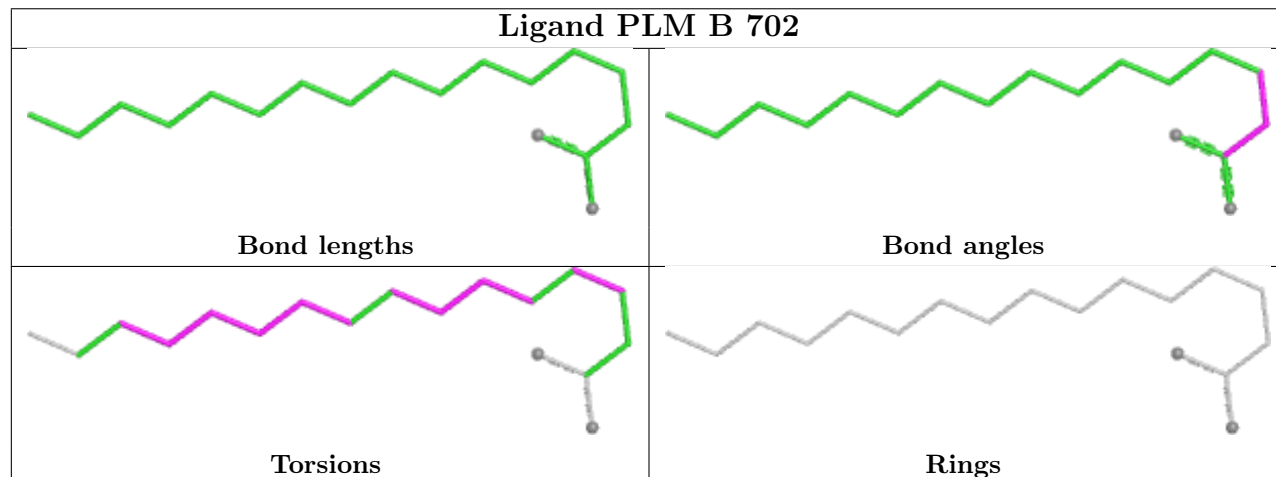


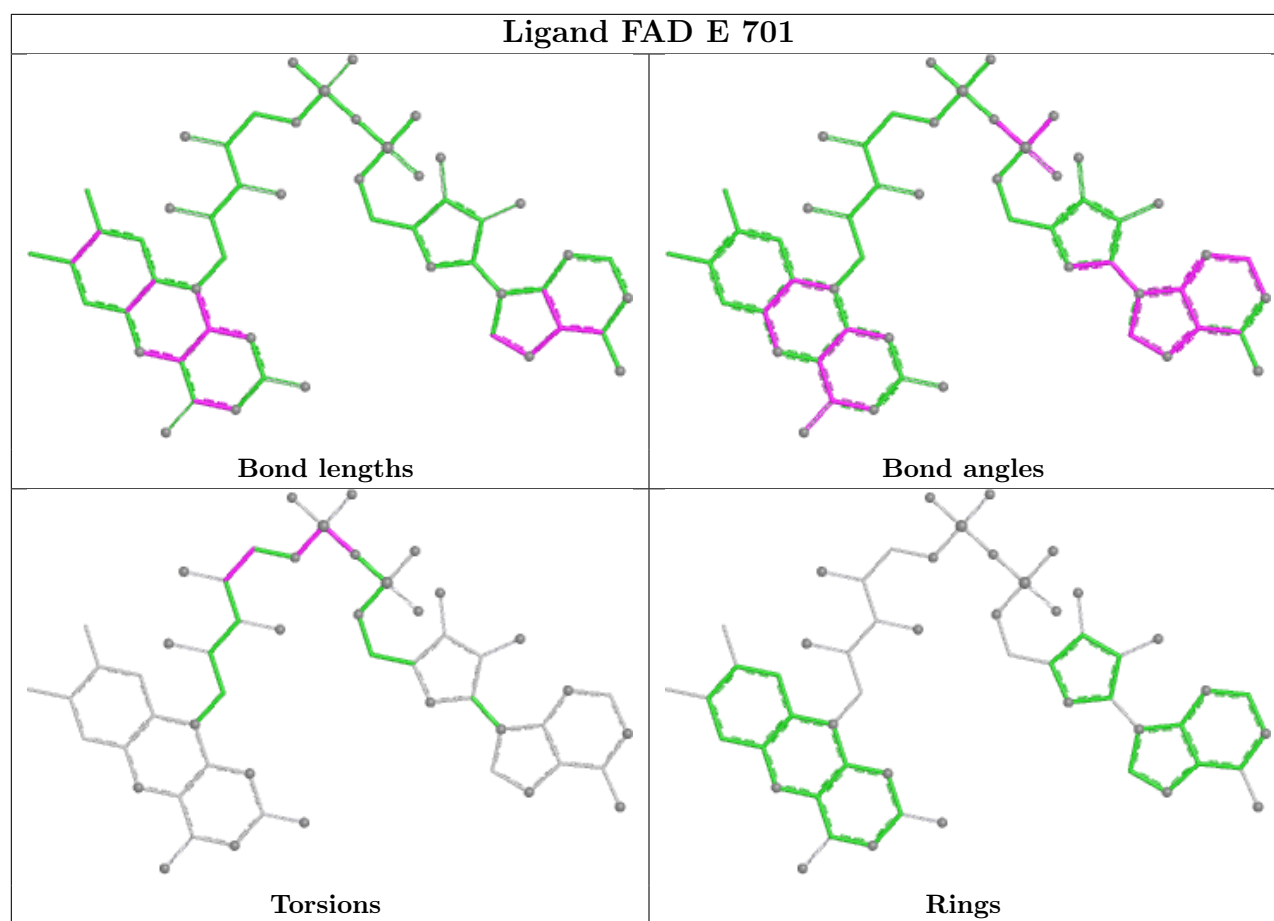


Ligand FAD B 701

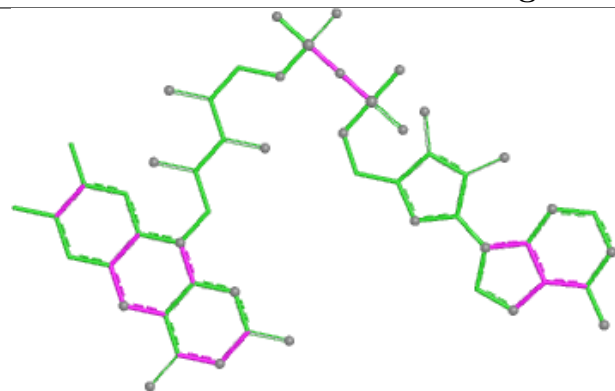


Ligand PLM B 702

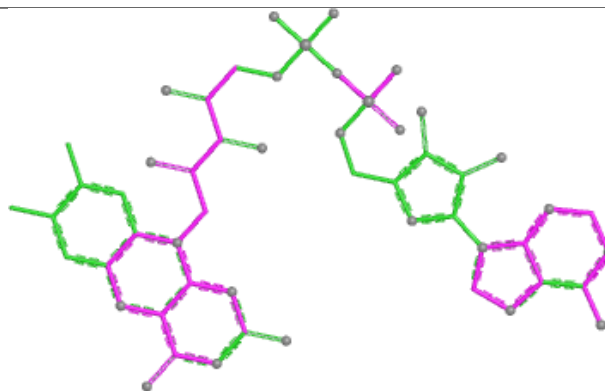




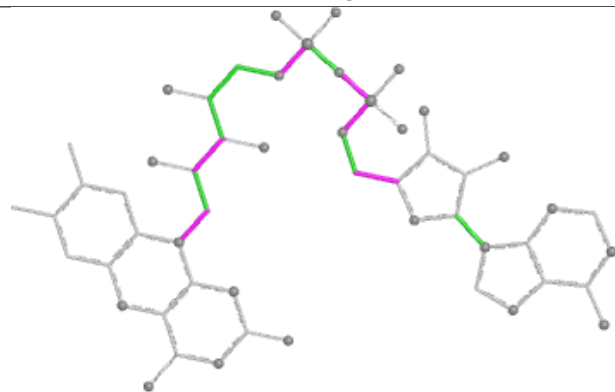
Ligand FAD F 701



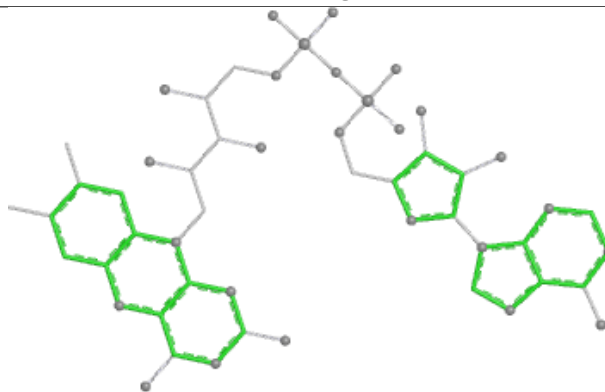
Bond lengths



Bond angles

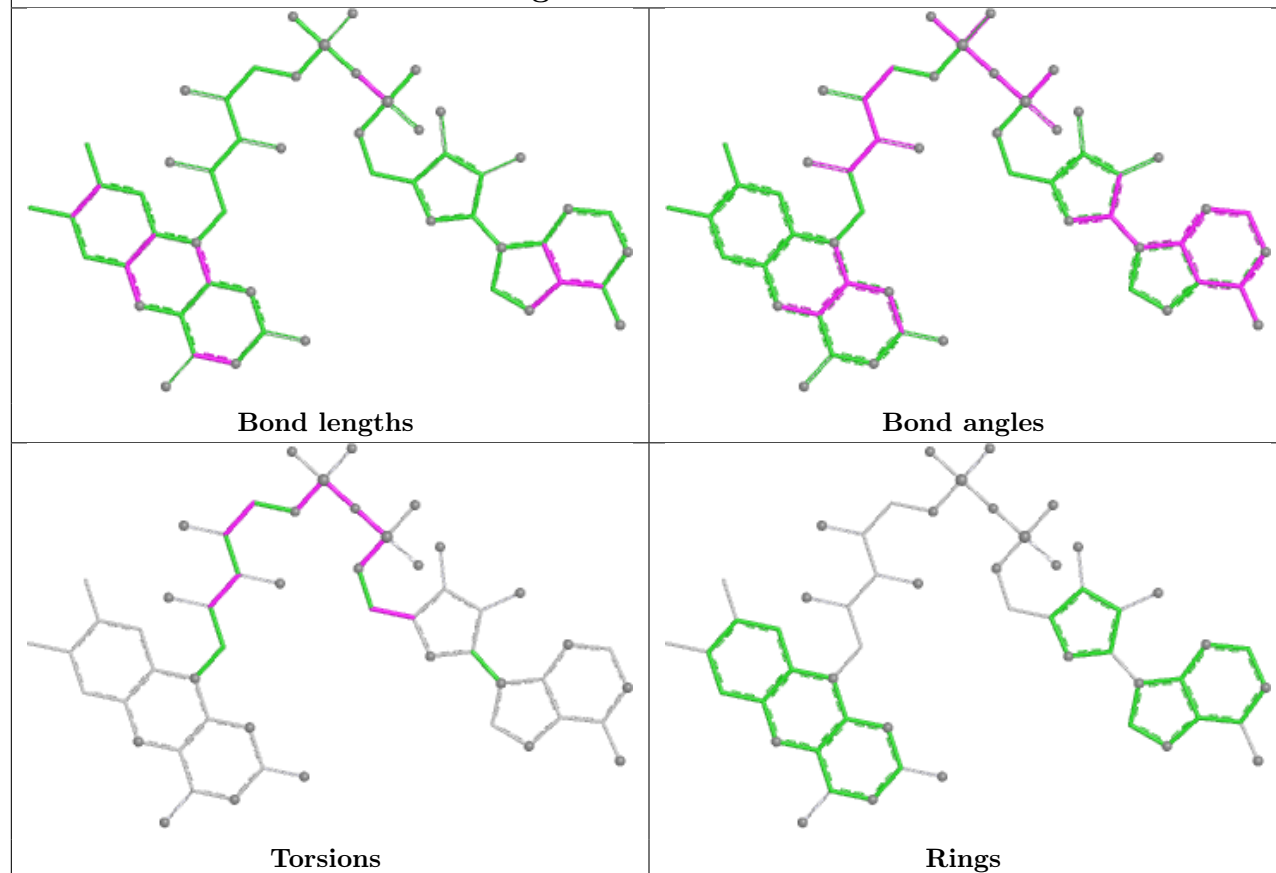


Torsions

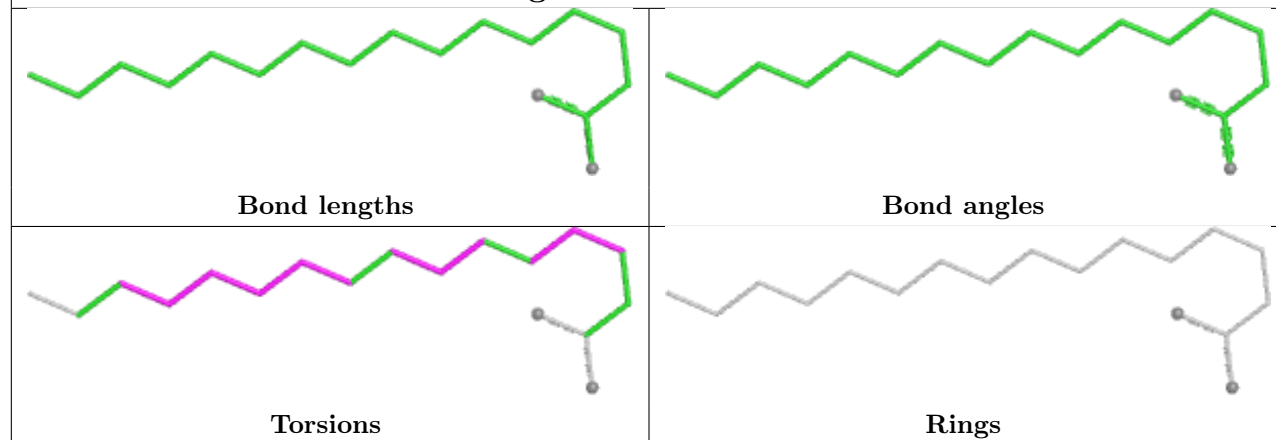


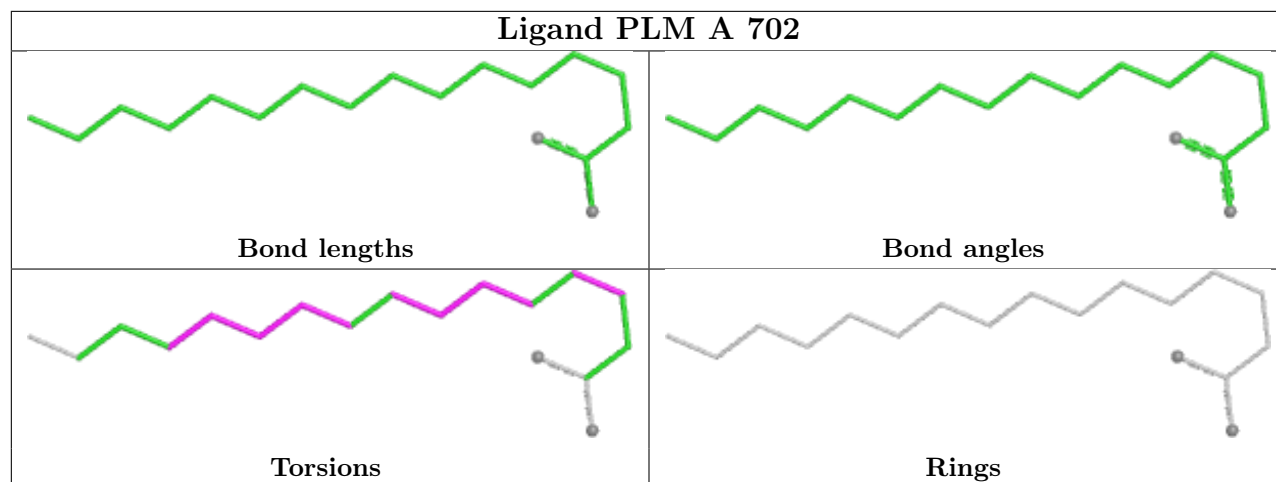
Rings

Ligand FAD D 701



Ligand PLM D 702





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	578/594 (97%)	-0.02	12 (2%)	63	42	20, 41, 74, 102	0
1	B	578/594 (97%)	0.08	13 (2%)	62	41	21, 43, 77, 119	0
1	C	578/594 (97%)	0.10	18 (3%)	51	31	22, 44, 79, 114	0
1	D	578/594 (97%)	0.14	13 (2%)	62	41	24, 48, 78, 132	0
1	E	578/594 (97%)	1.05	74 (12%)	7	4	46, 90, 127, 152	0
1	F	578/594 (97%)	1.00	69 (11%)	9	5	47, 86, 123, 170	0
All	All	3468/3564 (97%)	0.39	199 (5%)	29	16	20, 54, 112, 170	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	421	LEU	5.7
1	D	68	ILE	5.6
1	C	187	VAL	5.1
1	D	421	LEU	5.1
1	A	68	ILE	4.9
1	F	479	TRP	4.9
1	F	68	ILE	4.8
1	B	68	ILE	4.8
1	F	308	GLY	4.6
1	E	134	PHE	4.5
1	C	68	ILE	4.4
1	E	426	GLY	4.4
1	C	422	GLY	4.3
1	E	100	ASN	4.3
1	E	68	ILE	4.2
1	C	396	ASP	4.1
1	E	169	THR	3.8
1	F	426	GLY	3.8
1	A	409	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	421	LEU	3.7
1	F	433	ASP	3.6
1	F	551	LEU	3.6
1	D	187	VAL	3.6
1	A	421	LEU	3.6
1	F	263	THR	3.6
1	E	421	LEU	3.5
1	E	386	LEU	3.5
1	F	186	GLY	3.5
1	F	429	SER	3.4
1	E	628	ILE	3.3
1	F	480	PRO	3.3
1	F	365	GLY	3.3
1	B	187	VAL	3.3
1	F	419	TYR	3.2
1	F	549	GLY	3.2
1	F	124	VAL	3.2
1	F	438	VAL	3.2
1	C	409	GLY	3.2
1	F	233	HIS	3.2
1	E	430	THR	3.2
1	E	425	GLY	3.2
1	B	474	SER	3.2
1	D	62	ALA	3.2
1	B	409	GLY	3.2
1	E	479	TRP	3.2
1	A	186	GLY	3.1
1	E	403	HIS	3.1
1	D	245	LEU	3.1
1	B	422	GLY	3.1
1	A	429	SER	3.1
1	E	402	ASP	3.1
1	C	245	LEU	3.0
1	E	212	ALA	3.0
1	C	186	GLY	3.0
1	E	422	GLY	3.0
1	E	211	GLY	3.0
1	C	474	SER	2.9
1	E	206	ALA	2.9
1	E	213	TYR	2.9
1	F	395	TYR	2.9
1	E	98	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	118	ASP	2.9
1	F	432	CYS	2.9
1	E	281	LEU	2.9
1	F	430	THR	2.9
1	E	481	SER	2.8
1	E	139	ASP	2.8
1	E	477	LEU	2.8
1	E	167	SER	2.8
1	E	112	VAL	2.8
1	C	308	GLY	2.8
1	C	421	LEU	2.8
1	A	477	LEU	2.8
1	E	428	THR	2.8
1	E	469	PHE	2.8
1	E	409	GLY	2.8
1	F	436	ALA	2.8
1	E	89	VAL	2.7
1	E	245	LEU	2.7
1	F	226	ARG	2.7
1	E	551	LEU	2.7
1	B	426	GLY	2.7
1	E	474	SER	2.7
1	F	458	LEU	2.7
1	C	188	GLU	2.7
1	F	409	GLY	2.6
1	F	99	ALA	2.6
1	F	474	SER	2.6
1	F	538	ALA	2.6
1	A	245	LEU	2.6
1	F	251	PHE	2.6
1	E	401	SER	2.6
1	F	126	ILE	2.6
1	B	210	PRO	2.6
1	F	448	LEU	2.5
1	F	402	ASP	2.5
1	F	403	HIS	2.5
1	C	551	LEU	2.5
1	E	162	LEU	2.5
1	F	165	GLY	2.5
1	F	175	HIS	2.5
1	E	335	GLY	2.5
1	F	431	GLY	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	474	SER	2.5
1	E	480	PRO	2.5
1	F	557	VAL	2.5
1	D	409	GLY	2.5
1	F	110	VAL	2.5
1	F	267	MET	2.4
1	E	163	LEU	2.4
1	F	397	GLY	2.4
1	F	229	ASN	2.4
1	A	397	GLY	2.4
1	E	419	TYR	2.4
1	E	102	LEU	2.4
1	B	370	SER	2.4
1	E	621	THR	2.4
1	E	431	GLY	2.4
1	E	609	ASP	2.4
1	F	577	ILE	2.4
1	B	245	LEU	2.4
1	F	245	LEU	2.3
1	C	550	GLU	2.3
1	E	608	VAL	2.3
1	E	359	ALA	2.3
1	F	130	ILE	2.3
1	E	250	ASP	2.3
1	C	477	LEU	2.3
1	A	187	VAL	2.3
1	F	89	VAL	2.3
1	F	222	VAL	2.3
1	F	415	ALA	2.3
1	D	401	SER	2.3
1	B	188	GLU	2.3
1	E	101	ARG	2.3
1	F	235	ALA	2.3
1	F	260	GLY	2.3
1	E	276	MET	2.3
1	A	428	THR	2.3
1	F	246	THR	2.3
1	E	249	SER	2.3
1	E	210	PRO	2.2
1	E	576	ALA	2.2
1	F	575	ASN	2.2
1	E	393	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	459	ASP	2.2
1	E	567	ILE	2.2
1	D	477	LEU	2.2
1	F	232	LEU	2.2
1	D	208	PHE	2.2
1	E	280	TYR	2.2
1	E	271	GLY	2.2
1	E	470	ALA	2.2
1	F	237	PHE	2.2
1	F	552	PHE	2.2
1	A	430	THR	2.2
1	E	71	VAL	2.2
1	E	292	VAL	2.2
1	F	486	GLN	2.2
1	F	427	LEU	2.2
1	D	431	GLY	2.2
1	E	164	GLY	2.2
1	E	341	ALA	2.2
1	C	395	TYR	2.2
1	F	467	VAL	2.2
1	E	62	ALA	2.2
1	E	104	ALA	2.2
1	F	227	TYR	2.1
1	E	293	LEU	2.1
1	F	420	LEU	2.1
1	F	206	ALA	2.1
1	D	308	GLY	2.1
1	A	248	ASN	2.1
1	E	581	CYS	2.1
1	C	475	GLN	2.1
1	C	179	ALA	2.1
1	E	160	GLY	2.1
1	E	209	GLY	2.1
1	E	482	GLY	2.1
1	F	248	ASN	2.1
1	E	138	LEU	2.1
1	E	577	ILE	2.1
1	E	267	MET	2.1
1	F	280	TYR	2.1
1	F	481	SER	2.1
1	B	477	LEU	2.1
1	F	156	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	294	THR	2.1
1	F	384	ALA	2.1
1	E	618	GLY	2.1
1	F	401	SER	2.0
1	F	293	LEU	2.0
1	D	178	ALA	2.0
1	F	319	THR	2.0
1	E	279	GLN	2.0
1	E	509	PRO	2.0
1	C	65	VAL	2.0
1	E	227	TYR	2.0
1	B	396	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

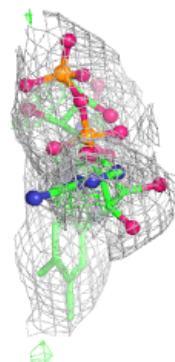
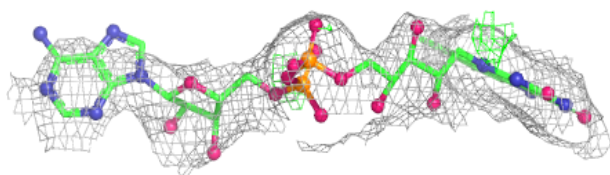
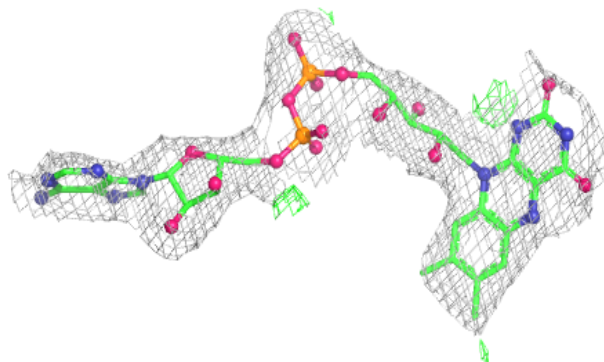
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	E	701	53/53	0.88	0.12	57,85,122,126	0
3	PLM	B	702	18/18	0.89	0.17	31,50,56,58	0
3	PLM	D	702	18/18	0.91	0.12	28,32,35,36	0
2	FAD	F	701	53/53	0.93	0.09	52,65,74,82	0
3	PLM	C	702	18/18	0.93	0.12	29,41,45,45	0
3	PLM	A	702	18/18	0.93	0.13	26,34,43,44	0
2	FAD	B	701	53/53	0.95	0.09	23,30,42,53	0
2	FAD	D	701	53/53	0.95	0.08	26,33,41,44	0
2	FAD	C	701	53/53	0.96	0.08	21,32,43,46	0
2	FAD	A	701	53/53	0.96	0.08	26,35,43,44	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.

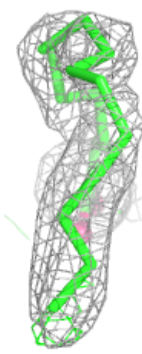
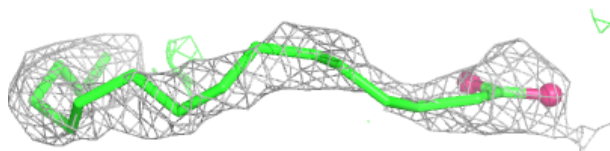
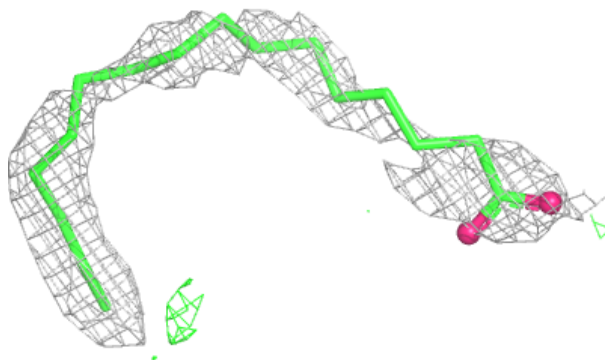
Electron density around FAD E 701:

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

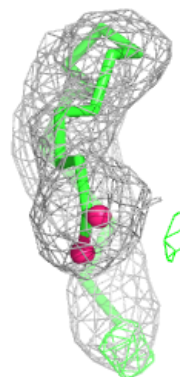
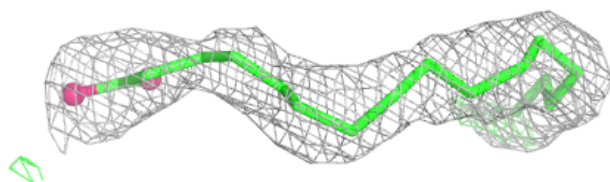
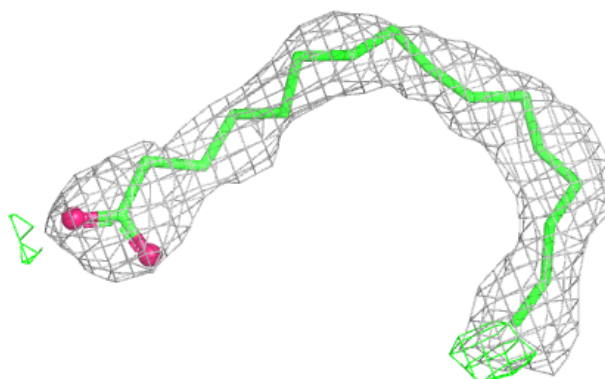


Electron density around PLM B 702:

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

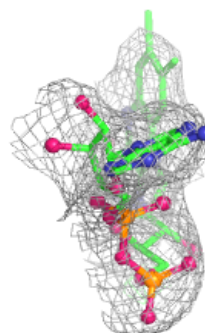
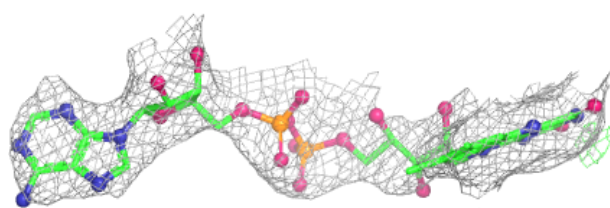
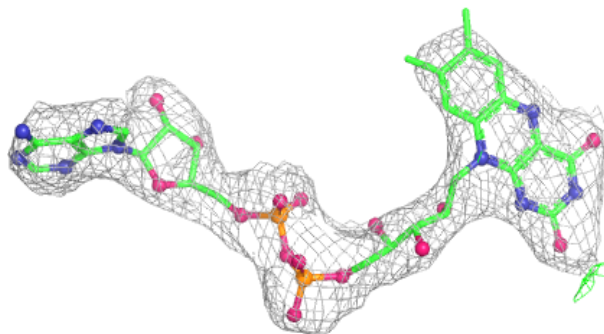
**Electron density around PLM D 702:**

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

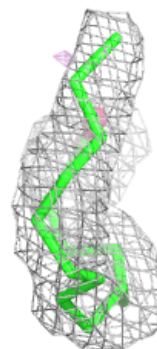
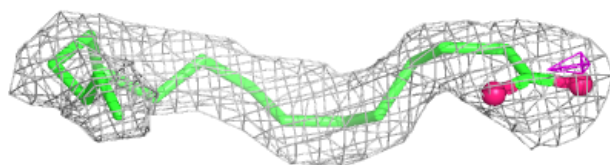
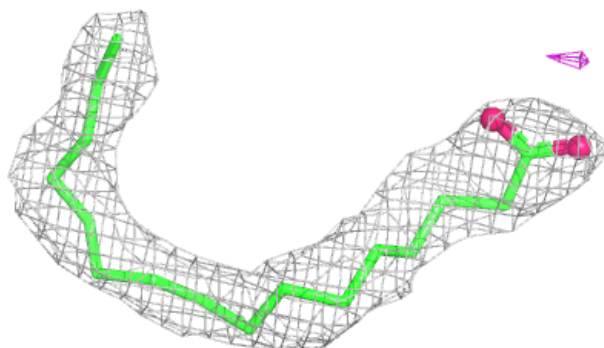


Electron density around FAD F 701:

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

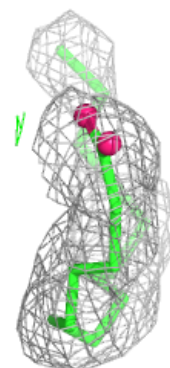
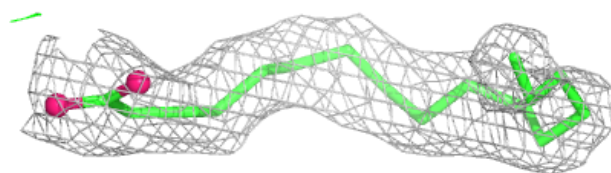
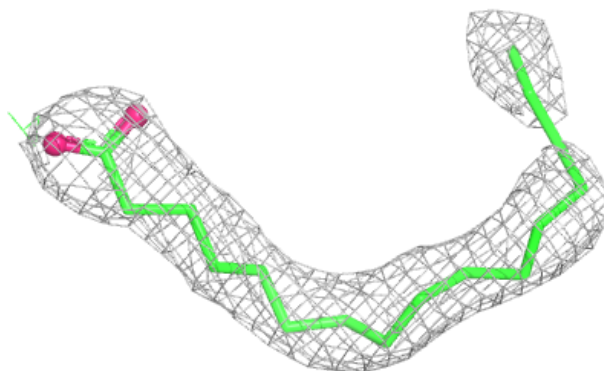
**Electron density around PLM C 702:**

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

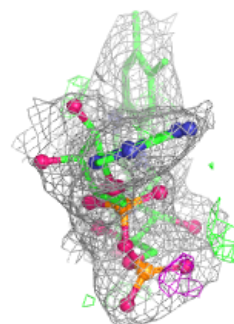
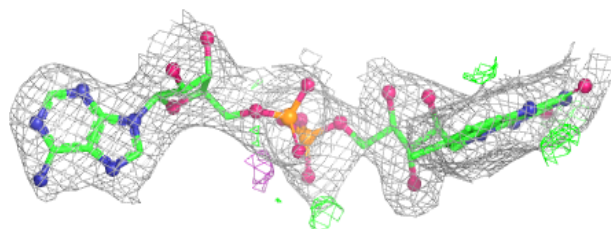
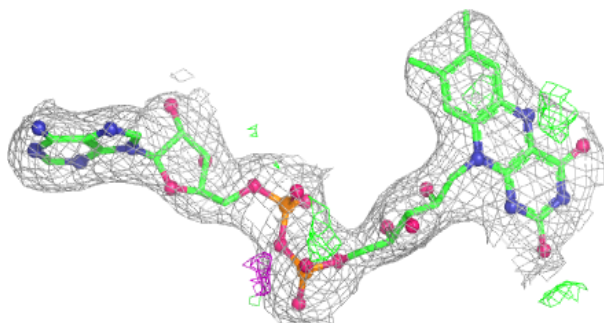


Electron density around PLM A 702:

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

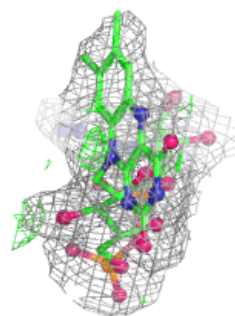
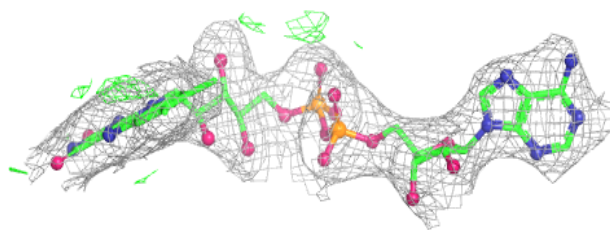
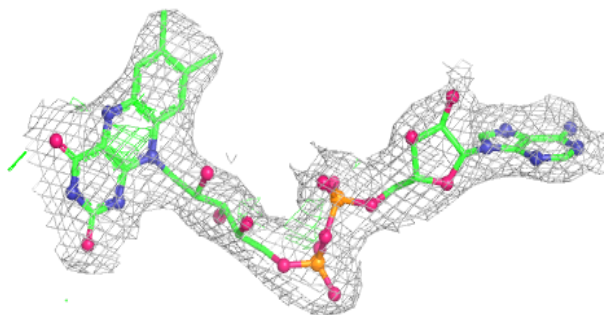
**Electron density around FAD B 701:**

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

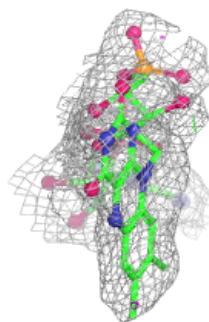
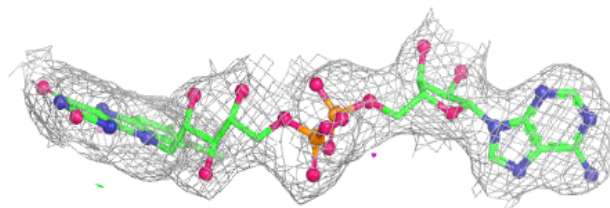
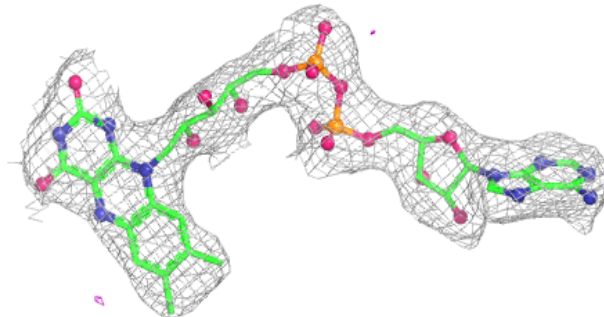


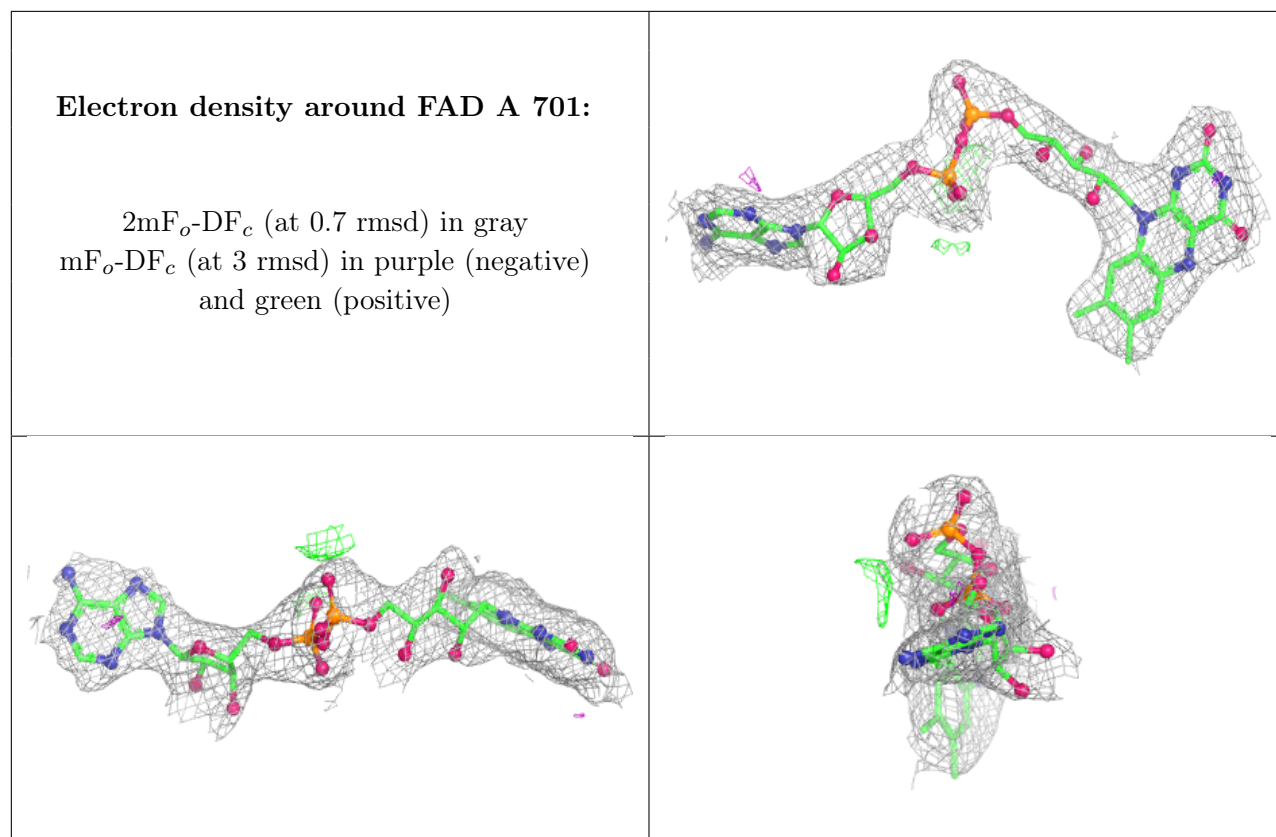
Electron density around FAD D 701:

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

**Electron density around FAD 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.