



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:31 PM UTC

PDB ID : 3AWI / pdb_00003awi
Title : Bifunctional tRNA modification enzyme MnmC from Escherichia coli
Authors : Kitamura, A.; Sengoku, T.; Nishimoto, M.; Yokoyama, S.; Bessho, Y.
Deposited on : 2011-03-23
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

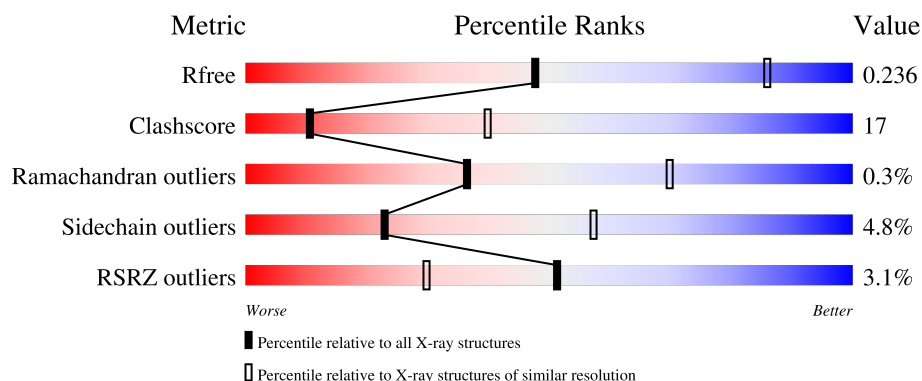
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	688	% 66% 23% 9%
1	B	688	69% 21% 9%
1	C	688	% 62% 28% 9%
1	D	688	% 58% 34% 9%
1	E	688	% 61% 27% 9%

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Mol	Chain	Length	Quality of chain
1	F	688	14% 54% 34% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30287 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 tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	628	Total	C	N	O	S	0	0	0
			4933	3125	867	914	27			
1	B	628	Total	C	N	O	S	0	0	0
			4933	3125	867	914	27			
1	C	628	Total	C	N	O	S	0	0	0
			4933	3125	867	914	27			
1	D	659	Total	C	N	O	S	0	0	0
			5188	3285	909	966	28			
1	E	628	Total	C	N	O	S	0	0	0
			4933	3125	867	914	27			
1	F	628	Total	C	N	O	S	0	0	0
			4933	3125	867	914	27			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P77182
A	-18	GLY	-	expression tag	UNP P77182
A	-17	SER	-	expression tag	UNP P77182
A	-16	SER	-	expression tag	UNP P77182
A	-15	HIS	-	expression tag	UNP P77182
A	-14	HIS	-	expression tag	UNP P77182
A	-13	HIS	-	expression tag	UNP P77182
A	-12	HIS	-	expression tag	UNP P77182
A	-11	HIS	-	expression tag	UNP P77182
A	-10	HIS	-	expression tag	UNP P77182
A	-9	SER	-	expression tag	UNP P77182
A	-8	SER	-	expression tag	UNP P77182
A	-7	GLY	-	expression tag	UNP P77182
A	-6	LEU	-	expression tag	UNP P77182
A	-5	VAL	-	expression tag	UNP P77182
A	-4	PRO	-	expression tag	UNP P77182

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ARG	-	expression tag	UNP P77182
A	-2	GLY	-	expression tag	UNP P77182
A	-1	SER	-	expression tag	UNP P77182
A	0	HIS	-	expression tag	UNP P77182
B	-19	MET	-	expression tag	UNP P77182
B	-18	GLY	-	expression tag	UNP P77182
B	-17	SER	-	expression tag	UNP P77182
B	-16	SER	-	expression tag	UNP P77182
B	-15	HIS	-	expression tag	UNP P77182
B	-14	HIS	-	expression tag	UNP P77182
B	-13	HIS	-	expression tag	UNP P77182
B	-12	HIS	-	expression tag	UNP P77182
B	-11	HIS	-	expression tag	UNP P77182
B	-10	HIS	-	expression tag	UNP P77182
B	-9	SER	-	expression tag	UNP P77182
B	-8	SER	-	expression tag	UNP P77182
B	-7	GLY	-	expression tag	UNP P77182
B	-6	LEU	-	expression tag	UNP P77182
B	-5	VAL	-	expression tag	UNP P77182
B	-4	PRO	-	expression tag	UNP P77182
B	-3	ARG	-	expression tag	UNP P77182
B	-2	GLY	-	expression tag	UNP P77182
B	-1	SER	-	expression tag	UNP P77182
B	0	HIS	-	expression tag	UNP P77182
C	-19	MET	-	expression tag	UNP P77182
C	-18	GLY	-	expression tag	UNP P77182
C	-17	SER	-	expression tag	UNP P77182
C	-16	SER	-	expression tag	UNP P77182
C	-15	HIS	-	expression tag	UNP P77182
C	-14	HIS	-	expression tag	UNP P77182
C	-13	HIS	-	expression tag	UNP P77182
C	-12	HIS	-	expression tag	UNP P77182
C	-11	HIS	-	expression tag	UNP P77182
C	-10	HIS	-	expression tag	UNP P77182
C	-9	SER	-	expression tag	UNP P77182
C	-8	SER	-	expression tag	UNP P77182
C	-7	GLY	-	expression tag	UNP P77182
C	-6	LEU	-	expression tag	UNP P77182
C	-5	VAL	-	expression tag	UNP P77182
C	-4	PRO	-	expression tag	UNP P77182
C	-3	ARG	-	expression tag	UNP P77182
C	-2	GLY	-	expression tag	UNP P77182

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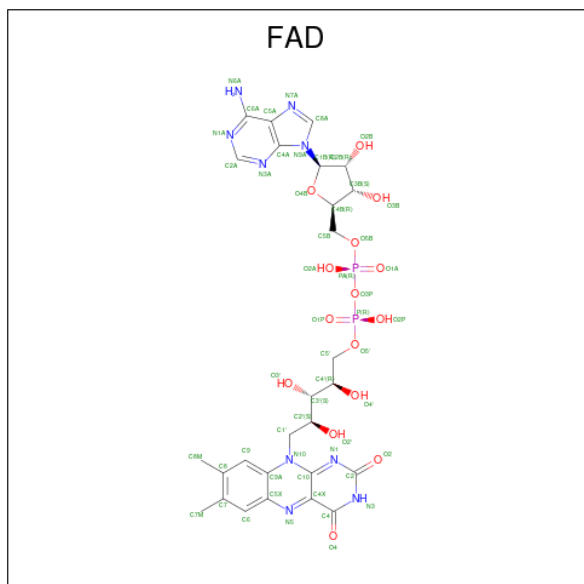
Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	SER	-	expression tag	UNP P77182
C	0	HIS	-	expression tag	UNP P77182
D	-19	MET	-	expression tag	UNP P77182
D	-18	GLY	-	expression tag	UNP P77182
D	-17	SER	-	expression tag	UNP P77182
D	-16	SER	-	expression tag	UNP P77182
D	-15	HIS	-	expression tag	UNP P77182
D	-14	HIS	-	expression tag	UNP P77182
D	-13	HIS	-	expression tag	UNP P77182
D	-12	HIS	-	expression tag	UNP P77182
D	-11	HIS	-	expression tag	UNP P77182
D	-10	HIS	-	expression tag	UNP P77182
D	-9	SER	-	expression tag	UNP P77182
D	-8	SER	-	expression tag	UNP P77182
D	-7	GLY	-	expression tag	UNP P77182
D	-6	LEU	-	expression tag	UNP P77182
D	-5	VAL	-	expression tag	UNP P77182
D	-4	PRO	-	expression tag	UNP P77182
D	-3	ARG	-	expression tag	UNP P77182
D	-2	GLY	-	expression tag	UNP P77182
D	-1	SER	-	expression tag	UNP P77182
D	0	HIS	-	expression tag	UNP P77182
E	-19	MET	-	expression tag	UNP P77182
E	-18	GLY	-	expression tag	UNP P77182
E	-17	SER	-	expression tag	UNP P77182
E	-16	SER	-	expression tag	UNP P77182
E	-15	HIS	-	expression tag	UNP P77182
E	-14	HIS	-	expression tag	UNP P77182
E	-13	HIS	-	expression tag	UNP P77182
E	-12	HIS	-	expression tag	UNP P77182
E	-11	HIS	-	expression tag	UNP P77182
E	-10	HIS	-	expression tag	UNP P77182
E	-9	SER	-	expression tag	UNP P77182
E	-8	SER	-	expression tag	UNP P77182
E	-7	GLY	-	expression tag	UNP P77182
E	-6	LEU	-	expression tag	UNP P77182
E	-5	VAL	-	expression tag	UNP P77182
E	-4	PRO	-	expression tag	UNP P77182
E	-3	ARG	-	expression tag	UNP P77182
E	-2	GLY	-	expression tag	UNP P77182
E	-1	SER	-	expression tag	UNP P77182
E	0	HIS	-	expression tag	UNP P77182

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP P77182
F	-18	GLY	-	expression tag	UNP P77182
F	-17	SER	-	expression tag	UNP P77182
F	-16	SER	-	expression tag	UNP P77182
F	-15	HIS	-	expression tag	UNP P77182
F	-14	HIS	-	expression tag	UNP P77182
F	-13	HIS	-	expression tag	UNP P77182
F	-12	HIS	-	expression tag	UNP P77182
F	-11	HIS	-	expression tag	UNP P77182
F	-10	HIS	-	expression tag	UNP P77182
F	-9	SER	-	expression tag	UNP P77182
F	-8	SER	-	expression tag	UNP P77182
F	-7	GLY	-	expression tag	UNP P77182
F	-6	LEU	-	expression tag	UNP P77182
F	-5	VAL	-	expression tag	UNP P77182
F	-4	PRO	-	expression tag	UNP P77182
F	-3	ARG	-	expression tag	UNP P77182
F	-2	GLY	-	expression tag	UNP P77182
F	-1	SER	-	expression tag	UNP P77182
F	0	HIS	-	expression tag	UNP P77182

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



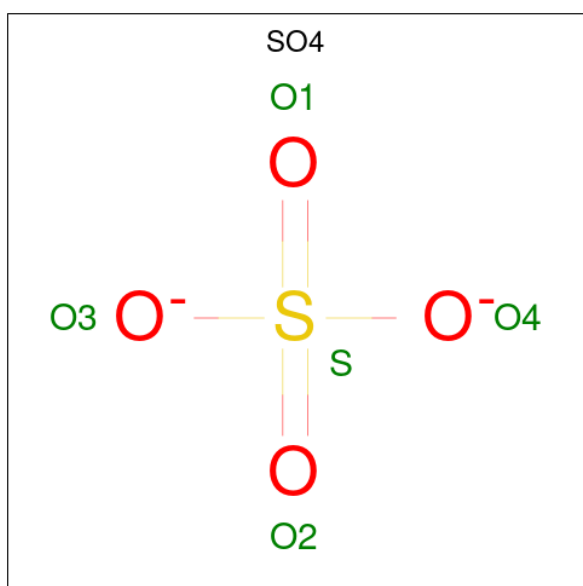
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O S	0	0
			5	4 1		
3	A	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	B	1	Total	O S	0	0
			5	4 1		
3	C	1	Total	O S	0	0
			5	4 1		
3	C	1	Total	O S	0	0
			5	4 1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

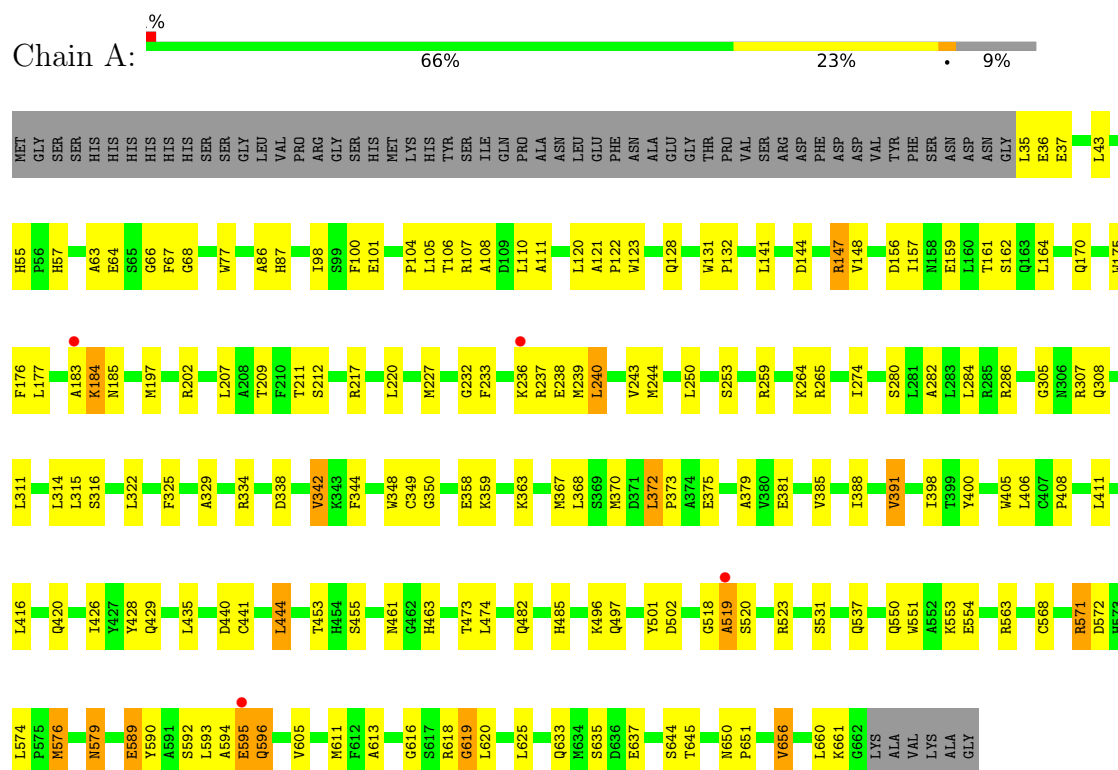
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	17	Total	O	0	0
			17	17		
4	B	11	Total	O	0	0
			11	11		
4	C	27	Total	O	0	0
			27	27		
4	D	5	Total	O	0	0
			5	5		
4	E	1	Total	O	0	0
			1	1		

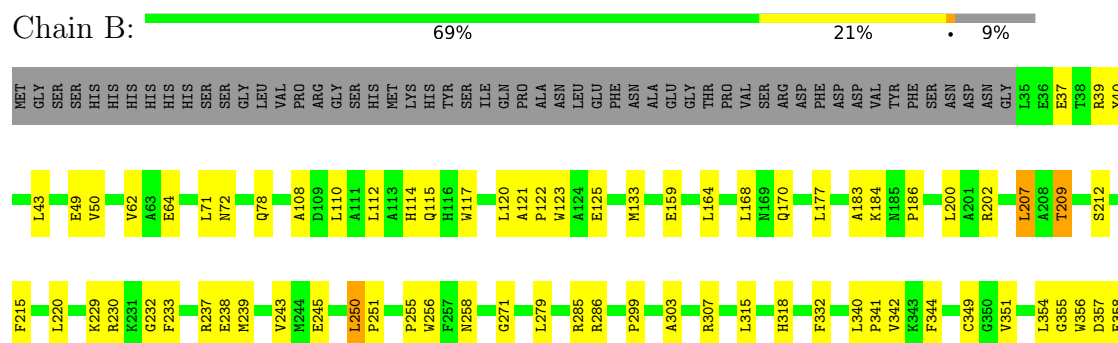
3 Residue-property plots

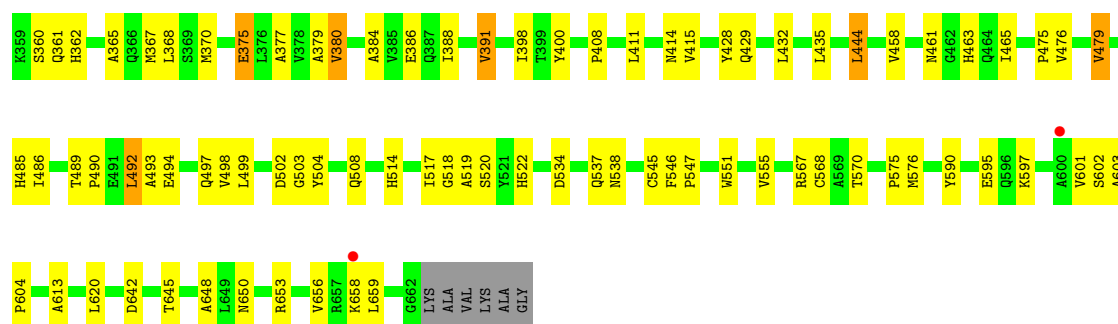
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC

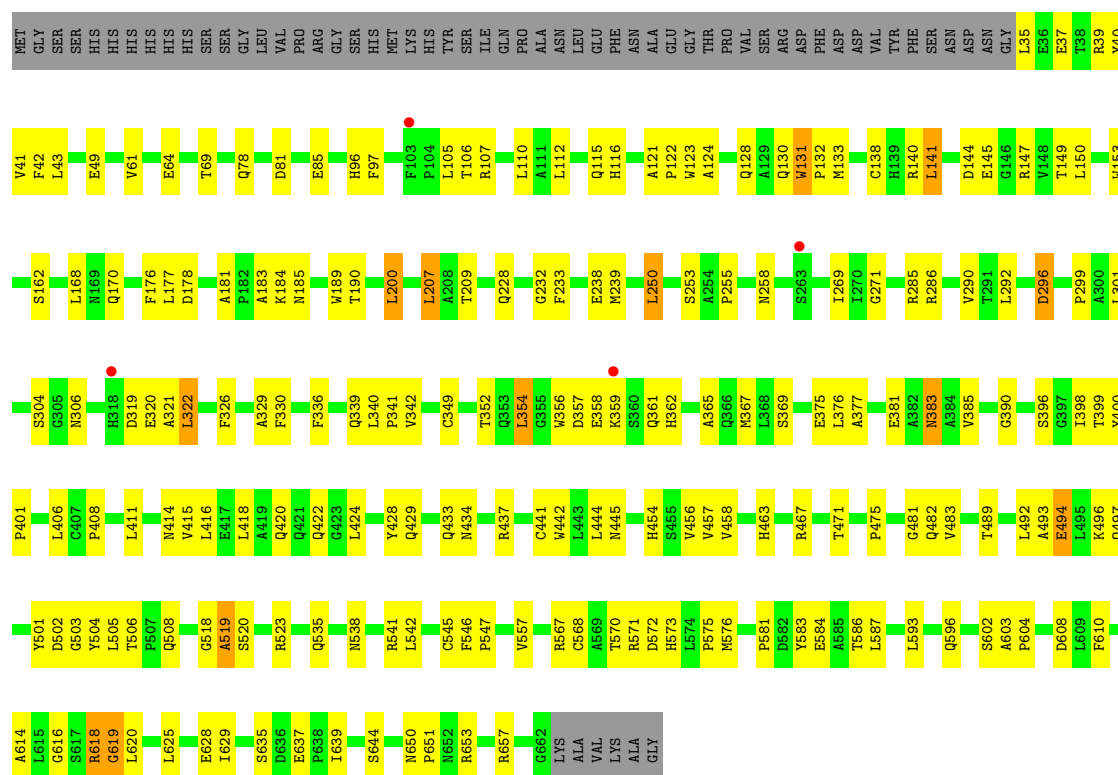


- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC

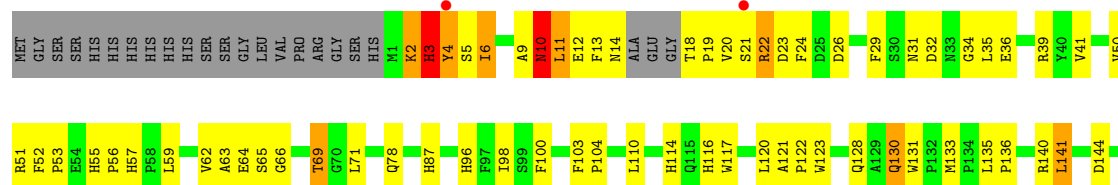


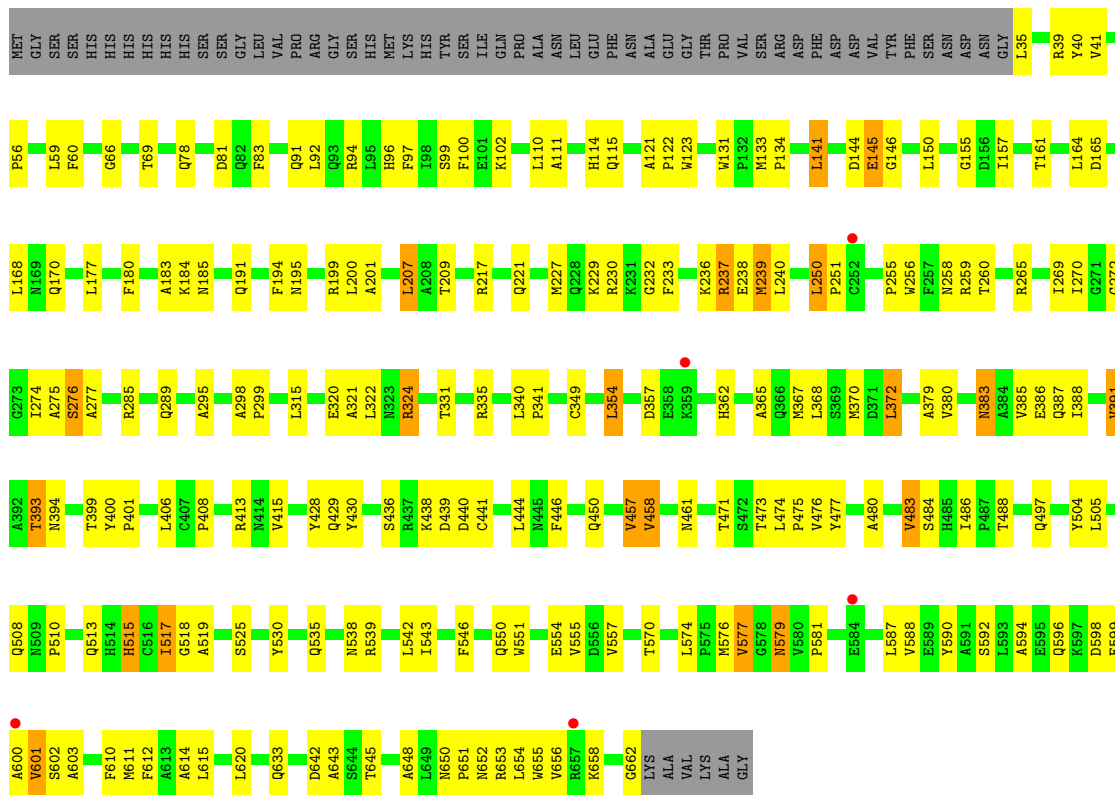


- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mmmC

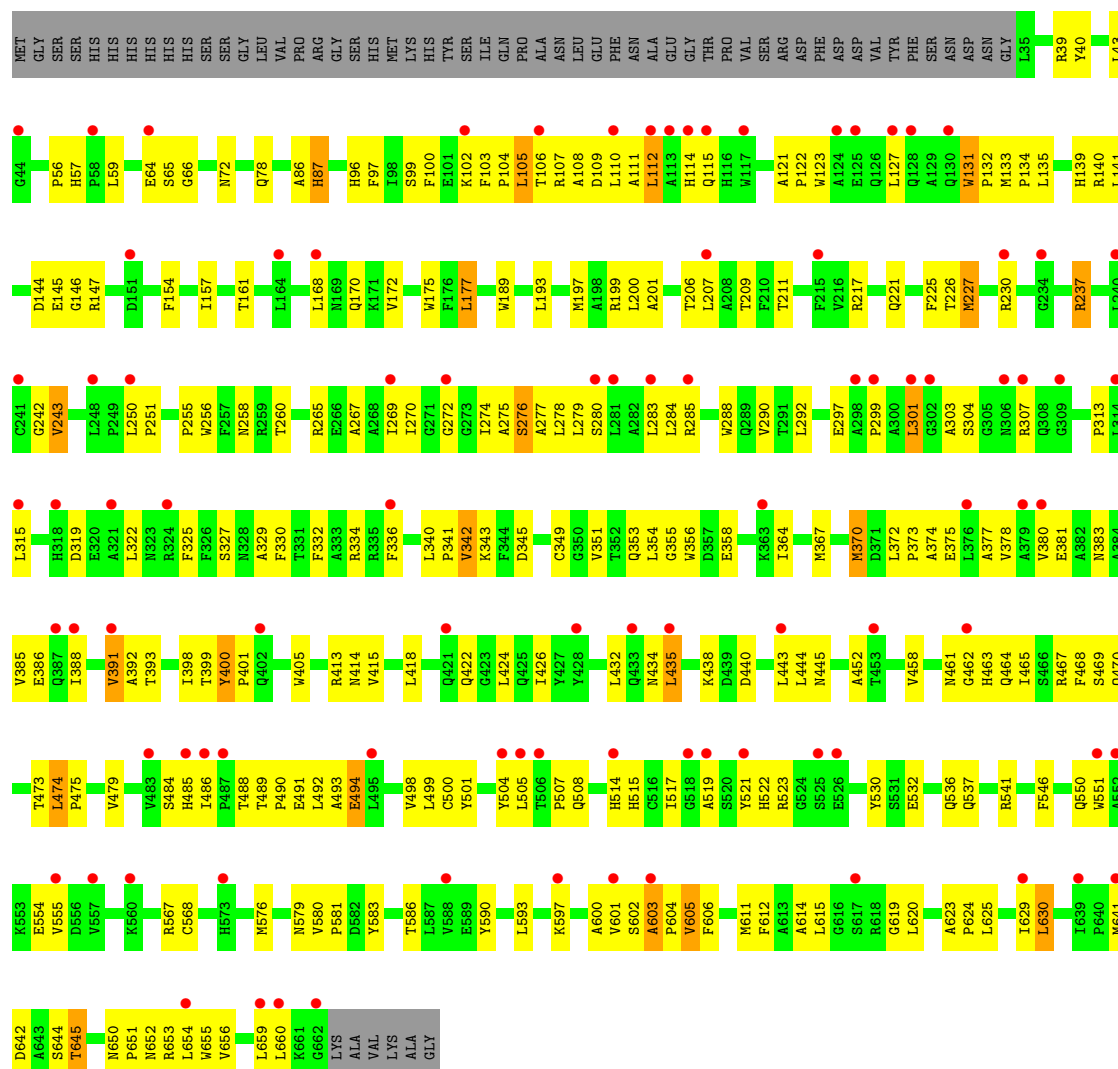


- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mmmC





- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mmmC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.14Å 243.02Å 175.53Å 90.00° 90.42° 90.00°	Depositor
Resolution (Å)	46.07 – 3.00 46.07 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.07-3.00) 95.3 (46.07-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.204 , 0.251 0.196 , 0.236	Depositor DCC
R_{free} test set	2002 reflections (1.15%)	wwPDB-VP
Wilson B-factor (Å ²)	50.0	Xtriage
Anisotropy	0.355	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.033 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	30287	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.27% 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: FAD, SO4

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	0.40	0/5060	0.85	12/6883 (0.2%)
1	B	0.41	0/5060	0.84	7/6883 (0.1%)
1	C	0.40	0/5060	0.87	12/6883 (0.2%)
1	D	0.36	0/5322	0.85	9/7238 (0.1%)
1	E	0.35	0/5060	0.80	5/6883 (0.1%)
1	F	0.32	0/5060	0.81	11/6883 (0.2%)
All	All	0.37	0/30622	0.84	56/41653 (0.1%)

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	D	0	1

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	LEU	CA-C-N	7.96	127.25	118.97
1	B	250	LEU	C-N-CA	7.96	127.25	118.97
1	C	250	LEU	CA-C-N	7.57	126.84	118.97
1	C	250	LEU	C-N-CA	7.57	126.84	118.97
1	A	250	LEU	CA-C-N	7.51	126.78	118.97
1	A	250	LEU	C-N-CA	7.51	126.78	118.97
1	D	250	LEU	CA-C-N	7.44	126.71	118.97
1	D	250	LEU	C-N-CA	7.44	126.71	118.97
1	A	571	ARG	N-CA-C	-7.07	101.71	110.41
1	D	603	ALA	CA-C-N	6.96	128.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	603	ALA	C-N-CA	6.96	128.54	119.84
1	C	494	GLU	N-CA-C	-6.63	105.19	113.28
1	F	603	ALA	CA-C-N	6.46	127.92	119.84
1	F	603	ALA	C-N-CA	6.46	127.92	119.84
1	C	185	ASN	N-CA-C	6.43	118.02	108.76
1	B	503	GLY	N-CA-C	-6.42	104.25	111.63
1	C	322	LEU	N-CA-C	-6.38	103.84	111.69
1	B	546	PHE	CA-C-N	6.34	126.82	119.47
1	B	546	PHE	C-N-CA	6.34	126.82	119.47
1	A	619	GLY	N-CA-C	6.15	120.08	112.64
1	F	494	GLU	N-CA-C	-6.06	105.89	113.28
1	E	131	TRP	CA-C-N	6.05	126.40	119.92
1	E	131	TRP	C-N-CA	6.05	126.40	119.92
1	A	502	ASP	N-CA-C	-6.04	103.85	112.13
1	A	613	ALA	N-CA-C	6.04	116.53	108.38
1	D	613	ALA	N-CA-C	5.91	116.36	108.38
1	A	441	CYS	N-CA-C	5.90	115.89	108.45
1	C	41	VAL	N-CA-C	5.87	116.00	110.30
1	F	105	LEU	N-CA-C	5.86	120.55	113.17
1	C	131	TRP	CA-C-N	5.62	125.81	120.31
1	C	131	TRP	C-N-CA	5.62	125.81	120.31
1	A	185	ASN	N-CA-C	5.61	116.83	108.76
1	A	131	TRP	CA-C-N	5.53	125.84	119.92
1	A	131	TRP	C-N-CA	5.53	125.84	119.92
1	F	131	TRP	CA-C-N	5.53	125.73	120.31
1	F	131	TRP	C-N-CA	5.53	125.73	120.31
1	C	619	GLY	N-CA-C	5.52	119.32	112.64
1	B	492	LEU	N-CA-C	-5.48	103.29	110.53
1	F	619	GLY	N-CA-C	5.42	119.44	112.83
1	C	471	THR	N-CA-C	5.41	119.99	113.17
1	A	426	ILE	N-CA-C	5.34	115.64	108.17
1	E	250	LEU	CA-C-N	5.32	125.38	119.32
1	E	250	LEU	C-N-CA	5.32	125.38	119.32
1	F	546	PHE	CA-C-N	5.31	124.64	118.85
1	F	546	PHE	C-N-CA	5.31	124.64	118.85
1	D	179	GLY	N-CA-C	-5.30	103.51	110.29
1	D	87	HIS	CA-C-N	5.17	124.79	119.05
1	D	87	HIS	C-N-CA	5.17	124.79	119.05
1	C	400	TYR	CA-C-N	5.07	124.73	119.56
1	C	400	TYR	C-N-CA	5.07	124.73	119.56
1	F	400	TYR	CA-C-N	5.06	124.67	119.05
1	F	400	TYR	C-N-CA	5.06	124.67	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	318	HIS	N-CA-C	5.05	117.90	111.69
1	D	494	GLU	N-CA-C	-5.02	106.84	113.17
1	A	108	ALA	N-CA-C	-5.01	105.29	111.40
1	E	588	VAL	N-CA-C	5.00	115.67	110.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	3	HIS	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	4933	0	4777	119	0
1	B	4933	0	4777	119	0
1	C	4933	0	4777	149	0
1	D	5188	0	5004	224	0
1	E	4933	0	4777	163	0
1	F	4933	0	4777	239	0
2	A	53	0	31	6	0
2	B	53	0	31	5	0
2	C	53	0	31	7	0
2	D	53	0	31	4	0
2	E	53	0	31	2	0
2	F	53	0	31	4	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	17	0	0	1	0
4	B	11	0	0	1	0
4	C	27	0	0	2	0
4	D	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
All	All	30287	0	29075	997	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (997) 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:324:ARG:HH11	1:E:324:ARG:HG2	1.07	1.19
1:D:334:ARG:HG3	1:D:334:ARG:HH11	1.04	1.16
1:C:271:GLY:HA3	1:C:292:LEU:HD11	1.41	1.03
1:D:354:LEU:HD22	1:D:393:THR:HG21	1.40	1.01
1:A:595:GLU:HA	1:E:477:TYR:HB3	1.38	1.01
1:C:519:ALA:HB3	1:C:538:ASN:OD1	1.61	1.00
1:D:21:SER:HB2	1:D:26:ASP:H	1.23	0.99
1:E:385:VAL:HG21	1:E:393:THR:HG22	1.45	0.98
1:F:475:PRO:HG2	1:F:576:MET:HE1	1.49	0.93
1:D:136:PRO:HB2	1:D:324:ARG:HH22	1.35	0.91
1:C:650:ASN:O	1:C:653:ARG:HG3	1.73	0.89
1:A:314:LEU:HB2	1:A:618:ARG:HE	1.37	0.88
1:C:475:PRO:HG2	1:C:576:MET:HE1	1.56	0.87
1:F:392:ALA:O	1:F:551:TRP:HH2	1.58	0.86
1:F:170:GLN:HA	1:F:201:ALA:O	1.76	0.86
1:E:217:ARG:HB2	1:E:240:LEU:HD21	1.57	0.86
1:D:334:ARG:HG3	1:D:334:ARG:NH1	1.80	0.85
1:D:618:ARG:HG3	1:D:618:ARG:HH11	1.41	0.85
1:B:230:ARG:HD3	1:B:239:MET:HE3	1.60	0.84
1:F:270:ILE:HG22	1:F:461:ASN:HB3	1.60	0.83
1:C:618:ARG:HH11	1:C:618:ARG:CG	1.92	0.82
1:D:518:GLY:HA3	1:D:538:ASN:CG	2.03	0.82
1:D:9:ALA:HB2	1:D:103:PHE:HB3	1.61	0.82
1:F:39:ARG:HG2	1:F:43:LEU:HD12	1.62	0.82
1:F:434:ASN:HB3	1:F:445:ASN:HB2	1.61	0.82
1:A:620:LEU:HG	2:A:901:FAD:O2	1.80	0.82
1:B:517:ILE:HG12	1:B:518:GLY:H	1.45	0.81
1:F:284:LEU:HD23	1:F:422:GLN:HB2	1.61	0.81
1:D:199:ARG:HG3	1:D:250:LEU:HD13	1.62	0.81
1:B:475:PRO:HG2	1:B:576:MET:HE1	1.61	0.80
1:E:324:ARG:HG2	1:E:324:ARG:NH1	1.85	0.79
1:D:270:ILE:HG22	1:D:461:ASN:HB3	1.63	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:ASP:OD1	1:F:106:THR:HG21	1.83	0.79
1:D:21:SER:CB	1:D:26:ASP:H	1.95	0.79
1:B:177:LEU:HB3	1:B:209:THR:HG23	1.65	0.78
1:C:519:ALA:HB1	1:C:541:ARG:NH2	1.98	0.78
1:E:59:LEU:HD11	1:E:96:HIS:HB2	1.65	0.78
1:F:66:GLY:HA2	1:F:100:PHE:O	1.83	0.78
1:D:489:THR:HB	1:D:490:PRO:HD2	1.66	0.77
1:F:580:VAL:O	1:F:605:VAL:HA	1.85	0.77
1:C:37:GLU:HB2	1:C:233:PHE:CE2	2.20	0.77
1:D:530:TYR:OH	1:D:560:LYS:HD3	1.85	0.76
1:E:535:GLN:HG3	1:E:557:VAL:CG1	2.15	0.76
1:F:508:GLN:HB3	1:F:515:HIS:NE2	2.01	0.76
1:A:388:ILE:HG22	1:A:497:GLN:OE1	1.86	0.76
1:C:618:ARG:HH11	1:C:618:ARG:HG3	1.49	0.76
1:B:518:GLY:HA3	1:B:538:ASN:CG	2.11	0.76
1:E:255:PRO:O	1:E:258:ASN:HB2	1.86	0.76
1:F:59:LEU:HD11	1:F:96:HIS:HB2	1.68	0.75
1:D:114:HIS:HD2	1:D:128:GLN:HE21	1.32	0.75
1:D:517:ILE:HG12	1:D:518:GLY:H	1.52	0.75
1:C:377:ALA:HB1	1:C:398:ILE:HD11	1.69	0.75
1:D:66:GLY:HA2	1:D:100:PHE:O	1.87	0.74
1:E:146:GLY:HA3	1:E:285:ARG:HD2	1.68	0.74
1:D:136:PRO:HB2	1:D:324:ARG:NH2	2.03	0.74
1:B:183:ALA:O	1:B:184:LYS:HB3	1.88	0.74
1:E:157:ILE:O	1:E:161:THR:HG23	1.88	0.74
1:D:380:VAL:HG21	1:D:388:ILE:HD12	1.70	0.74
1:D:618:ARG:HH11	1:D:618:ARG:CG	2.00	0.73
1:D:508:GLN:HB3	1:D:515:HIS:NE2	2.04	0.73
1:E:408:PRO:HB3	1:E:620:LEU:HD21	1.71	0.72
1:F:391:VAL:HG13	1:F:551:TRP:CZ2	2.24	0.72
1:F:604:PRO:HG2	1:F:605:VAL:HG23	1.72	0.72
1:E:232:GLY:H	1:E:238:GLU:HA	1.54	0.72
1:F:269:ILE:HG13	1:F:458:VAL:HB	1.71	0.72
1:A:236:LYS:HG2	1:A:237:ARG:H	1.52	0.71
1:D:59:LEU:HD11	1:D:96:HIS:HB2	1.72	0.71
1:A:217:ARG:HB2	1:A:240:LEU:HD21	1.71	0.71
1:F:315:LEU:HB2	1:F:367:MET:HE3	1.71	0.71
1:D:232:GLY:HA3	1:D:237:ARG:O	1.91	0.71
1:F:307:ARG:HB2	1:F:485:HIS:HE1	1.55	0.70
1:B:40:TYR:CE2	1:B:239:MET:HE2	2.27	0.70
1:E:170:GLN:HA	1:E:201:ALA:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:550:GLN:HG2	1:E:551:TRP:N	2.06	0.70
1:D:570:THR:HG21	1:D:574:LEU:O	1.92	0.70
1:F:435:LEU:HD12	1:F:435:LEU:O	1.90	0.70
1:A:482:GLN:H	1:A:520:SER:HB3	1.54	0.70
1:E:517:ILE:HG12	1:E:518:GLY:H	1.55	0.70
1:D:620:LEU:HB2	2:D:901:FAD:O2	1.91	0.70
1:F:576:MET:HE2	1:F:653:ARG:HH12	1.56	0.70
1:B:186:PRO:HG3	1:D:253:SER:HB3	1.72	0.70
1:C:207:LEU:C	1:C:207:LEU:HD12	2.17	0.70
1:A:620:LEU:HG	2:A:901:FAD:C2	2.22	0.69
1:C:301:LEU:HD22	1:F:112:LEU:HG	1.74	0.69
1:C:433:GLN:HB3	1:F:373:PRO:HA	1.74	0.69
1:E:518:GLY:HA3	1:E:538:ASN:CG	2.18	0.69
1:D:133:MET:HE1	1:D:376:LEU:HB2	1.75	0.69
1:C:140:ARG:C	1:C:141:LEU:HD23	2.18	0.69
1:F:227:MET:HE2	1:F:242:GLY:HA3	1.74	0.69
1:F:550:GLN:HG2	1:F:551:TRP:HE3	1.56	0.69
1:D:354:LEU:CD2	1:D:393:THR:HG21	2.21	0.69
1:E:550:GLN:HG2	1:E:551:TRP:H	1.58	0.69
1:C:492:LEU:O	1:C:493:ALA:HB3	1.92	0.69
1:E:504:TYR:CE2	1:E:519:ALA:HB2	2.27	0.68
1:B:315:LEU:HD12	1:B:367:MET:HE3	1.75	0.68
1:F:237:ARG:H	1:F:237:ARG:HD2	1.57	0.68
1:D:41:VAL:HA	1:D:239:MET:HE1	1.76	0.68
1:C:434:ASN:HB3	1:C:445:ASN:HB2	1.76	0.68
1:F:351:VAL:HG22	1:F:498:VAL:HB	1.77	0.67
1:D:21:SER:HB2	1:D:26:ASP:N	2.03	0.67
1:D:488:THR:OG1	1:D:493:ALA:HB2	1.94	0.67
1:D:173:ASP:OD2	1:D:202:ARG:HD3	1.94	0.67
1:D:352:THR:HG23	1:D:497:GLN:OE1	1.95	0.67
1:D:491:GLU:HG2	1:D:551:TRP:HB3	1.75	0.67
1:E:612:PHE:HE2	1:E:615:LEU:HD21	1.59	0.67
1:F:276:SER:O	1:F:280:SER:HB2	1.95	0.67
1:D:385:VAL:HG11	1:D:393:THR:HG23	1.76	0.67
1:C:593:LEU:HA	1:C:596:GLN:HB3	1.76	0.67
1:F:484:SER:HB2	1:F:517:ILE:HG23	1.78	0.66
1:C:144:ASP:HB3	1:C:147:ARG:HB2	1.78	0.66
1:A:107:ARG:HA	1:A:110:LEU:HB3	1.77	0.66
1:B:367:MET:HE1	1:B:400:TYR:OH	1.94	0.66
1:D:12:GLU:H	1:D:20:VAL:HG12	1.61	0.66
1:C:381:GLU:HG2	1:C:383:ASN:HD22	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:HD23	1:D:39:ARG:NH2	2.12	0.65
1:D:4:TYR:C	1:D:4:TYR:CD2	2.73	0.65
1:B:232:GLY:N	1:B:238:GLU:HA	2.11	0.65
1:F:227:MET:CE	1:F:242:GLY:HA3	2.26	0.65
1:A:144:ASP:HB3	1:A:147:ARG:HB2	1.78	0.65
1:D:571:ARG:O	1:D:572:ASP:CG	2.39	0.65
1:E:476:VAL:HG12	1:E:570:THR:HG22	1.79	0.65
1:F:576:MET:H	1:F:614:ALA:HB3	1.59	0.65
1:A:350:GLY:HA3	1:A:497:GLN:HE21	1.60	0.65
1:E:295:ALA:O	1:E:429:GLN:HA	1.95	0.65
1:C:429:GLN:HB3	1:F:103:PHE:HB3	1.79	0.65
1:D:463:HIS:HA	1:D:568:CYS:HB2	1.78	0.64
1:F:462:GLY:O	1:F:465:ILE:HG23	1.97	0.64
1:D:314:LEU:HD22	1:D:618:ARG:NH1	2.12	0.64
1:B:492:LEU:O	1:B:493:ALA:HB3	1.97	0.64
1:C:523:ARG:HH22	1:C:571:ARG:NH2	1.94	0.64
1:D:13:PHE:HA	1:D:19:PRO:HA	1.80	0.64
1:D:19:PRO:HD2	1:D:29:PHE:CZ	2.33	0.64
1:D:486:ILE:HG12	1:D:515:HIS:HB2	1.80	0.64
1:D:461:ASN:HB2	2:D:901:FAD:C8A	2.28	0.64
1:C:583:TYR:O	1:C:587:LEU:HD12	1.98	0.64
1:F:655:TRP:O	1:F:659:LEU:HB2	1.97	0.64
1:A:550:GLN:NE2	1:A:553:LYS:HE3	2.13	0.64
1:A:474:LEU:HD22	1:A:576:MET:HE1	1.79	0.63
1:D:340:LEU:HD12	1:D:341:PRO:HD2	1.80	0.63
1:D:334:ARG:HH12	1:D:402:GLN:HB3	1.63	0.63
1:E:207:LEU:C	1:E:207:LEU:HD12	2.24	0.63
1:B:209:THR:O	1:B:239:MET:HB2	1.99	0.63
1:B:517:ILE:HG12	1:B:518:GLY:N	2.11	0.63
1:A:579:ASN:H	1:A:579:ASN:ND2	1.96	0.63
1:C:381:GLU:HG2	1:C:383:ASN:ND2	2.14	0.63
1:D:9:ALA:O	1:D:10:ASN:HB3	1.98	0.63
1:E:475:PRO:HG2	1:E:576:MET:HE1	1.80	0.63
1:D:20:VAL:HG22	1:D:21:SER:H	1.64	0.63
1:F:537:GLN:O	1:F:541:ARG:HG2	1.99	0.63
1:D:10:ASN:O	1:D:11:LEU:HD13	1.99	0.63
1:A:212:SER:HB3	1:A:238:GLU:O	1.99	0.63
1:B:408:PRO:HB3	1:B:620:LEU:HD21	1.81	0.63
1:F:612:PHE:HE1	1:F:615:LEU:HD11	1.64	0.63
1:D:29:PHE:HD2	1:D:31:ASN:H	1.46	0.63
1:D:492:LEU:O	1:D:493:ALA:HB3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:PHE:CE2	1:F:99:SER:HB2	2.34	0.63
1:F:464:GLN:HB3	1:F:467:ARG:HD3	1.80	0.63
1:D:352:THR:HG22	1:D:399:THR:OG1	1.99	0.62
1:F:297:GLU:CD	1:F:297:GLU:H	2.07	0.62
1:D:9:ALA:HB1	1:D:23:ASP:OD1	2.00	0.62
1:B:243:VAL:HG13	1:B:245:GLU:HG3	1.81	0.62
1:D:10:ASN:OD1	1:D:22:ARG:HG2	1.98	0.62
1:A:596:GLN:HA	1:A:596:GLN:NE2	2.14	0.62
1:F:435:LEU:CD2	1:F:468:PHE:HB3	2.30	0.62
1:B:122:PRO:HG2	1:B:123:TRP:CE3	2.34	0.62
1:D:658:LYS:HG3	1:D:659:LEU:N	2.15	0.62
1:C:482:GLN:H	1:C:520:SER:HB3	1.65	0.62
1:E:232:GLY:N	1:E:238:GLU:HA	2.15	0.61
1:C:255:PRO:O	1:C:258:ASN:HB2	1.99	0.61
1:D:13:PHE:O	1:D:14:ASN:HB3	2.00	0.61
1:D:35:LEU:HD11	1:D:120:LEU:HD11	1.81	0.61
1:C:575:PRO:O	1:C:653:ARG:NH2	2.34	0.61
1:E:144:ASP:C	1:E:145:GLU:HG2	2.24	0.61
1:F:87:HIS:N	1:F:87:HIS:CD2	2.68	0.61
1:F:135:LEU:HD13	1:F:327:SER:HB3	1.83	0.61
1:A:308:GLN:HG2	1:A:405:TRP:CE3	2.36	0.61
1:E:331:THR:HG22	1:E:335:ARG:NH1	2.14	0.61
1:E:386:GLU:HA	1:E:391:VAL:O	2.00	0.61
1:A:367:MET:HE1	1:A:400:TYR:OH	2.01	0.61
1:A:183:ALA:O	1:A:184:LYS:HB3	2.00	0.60
1:A:264:LYS:HD3	1:A:455:SER:HB3	1.83	0.60
1:E:504:TYR:HE2	1:E:519:ALA:HB2	1.66	0.60
1:F:65:SER:HA	1:F:157:ILE:HD12	1.82	0.60
1:F:354:LEU:HD21	1:F:385:VAL:HG11	1.83	0.60
1:A:435:LEU:CD2	1:A:444:LEU:HD22	2.31	0.60
1:C:124:ALA:O	1:C:128:GLN:HG3	2.01	0.60
1:F:461:ASN:OD1	1:F:465:ILE:HG22	2.02	0.60
1:C:584:GLU:HG2	1:F:381:GLU:HB3	1.83	0.60
1:B:432:LEU:HD21	1:B:435:LEU:HD13	1.82	0.60
1:B:576:MET:HG2	1:B:653:ARG:NH2	2.17	0.60
1:E:576:MET:HG2	1:E:653:ARG:HH12	1.66	0.60
1:E:471:THR:HB	1:E:474:LEU:HD12	1.83	0.60
1:D:78:GLN:HG3	1:D:123:TRP:CH2	2.36	0.60
1:D:114:HIS:CD2	1:D:128:GLN:HE21	2.17	0.59
1:D:228:GLN:HG2	1:D:229:LYS:O	2.01	0.59
1:B:232:GLY:H	1:B:238:GLU:HA	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LEU:HD13	1:D:117:TRP:CZ3	2.37	0.59
1:C:358:GLU:HG2	1:C:359:LYS:N	2.18	0.59
1:E:385:VAL:HG21	1:E:393:THR:CG2	2.26	0.59
1:F:550:GLN:HG2	1:F:551:TRP:H	1.66	0.59
1:E:367:MET:HE1	1:E:400:TYR:OH	2.02	0.59
1:B:463:HIS:HA	1:B:568:CYS:HB2	1.84	0.59
1:A:391:VAL:HG13	1:A:551:TRP:CE2	2.37	0.59
1:E:237:ARG:HG3	1:E:238:GLU:H	1.68	0.59
1:D:121:ALA:N	1:D:122:PRO:HD2	2.17	0.59
1:A:367:MET:O	1:A:370:MET:HG2	2.02	0.59
1:D:590:TYR:HB2	1:D:659:LEU:HD23	1.85	0.58
1:C:40:TYR:CE2	1:C:239:MET:HE2	2.38	0.58
1:C:349:CYS:O	1:C:497:GLN:HG2	2.02	0.58
1:B:377:ALA:HB1	1:B:398:ILE:HD11	1.84	0.58
1:D:69:THR:O	1:D:114:HIS:HE1	1.87	0.58
1:F:274:ILE:HD13	1:F:620:LEU:HD23	1.84	0.58
1:D:317:LYS:HE3	1:D:318:HIS:CE1	2.39	0.58
1:E:354:LEU:HD22	1:E:393:THR:HG21	1.86	0.58
1:A:157:ILE:O	1:A:161:THR:HG23	2.03	0.58
1:A:485:HIS:HE1	4:A:674:HOH:O	1.86	0.58
1:E:458:VAL:HA	1:E:610:PHE:O	2.03	0.58
1:F:551:TRP:HA	1:F:554:GLU:HG3	1.85	0.58
1:A:444:LEU:HD23	1:A:444:LEU:N	2.19	0.58
1:B:37:GLU:HB2	1:B:233:PHE:CE2	2.39	0.58
1:B:255:PRO:HD2	1:B:256:TRP:CZ3	2.39	0.58
1:C:502:ASP:HB3	1:C:541:ARG:HG2	1.86	0.58
1:D:615:LEU:HD12	2:D:901:FAD:H5'2	1.86	0.58
1:F:193:LEU:O	1:F:197:MET:HG3	2.04	0.58
1:A:518:GLY:O	1:A:519:ALA:HB3	2.03	0.57
1:C:81:ASP:O	1:C:85:GLU:HG2	2.04	0.57
1:F:283:LEU:O	1:F:288:TRP:HB2	2.03	0.57
1:D:3:HIS:O	1:D:3:HIS:CG	2.57	0.57
1:D:51:ARG:O	1:D:55:HIS:HB2	2.04	0.57
1:F:356:TRP:H	1:F:356:TRP:CD1	2.23	0.57
1:B:255:PRO:O	1:B:258:ASN:HB2	2.04	0.57
1:D:367:MET:O	1:D:370:MET:HG2	2.04	0.57
1:D:550:GLN:CD	1:D:550:GLN:H	2.11	0.57
1:D:618:ARG:CG	1:D:618:ARG:NH1	2.65	0.57
1:A:106:THR:O	1:A:107:ARG:HB3	2.05	0.57
1:A:367:MET:HE2	1:A:398:ILE:HD13	1.85	0.57
1:A:461:ASN:HB2	2:A:901:FAD:C8A	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:650:ASN:OD1	1:E:651:PRO:HD2	2.04	0.57
1:F:479:VAL:O	1:F:567:ARG:HG2	2.04	0.57
1:F:370:MET:HE2	1:F:372:LEU:HD11	1.86	0.57
1:F:492:LEU:O	1:F:493:ALA:HB3	2.04	0.57
1:F:579:ASN:HB3	1:F:605:VAL:CG1	2.34	0.57
1:E:321:ALA:HA	1:E:645:THR:HG22	1.87	0.57
1:F:354:LEU:HD13	1:F:393:THR:HG21	1.86	0.57
1:A:207:LEU:HD12	1:A:207:LEU:C	2.30	0.57
1:F:290:VAL:HG12	1:F:424:LEU:HD13	1.86	0.57
1:D:157:ILE:O	1:D:161:THR:HG23	2.05	0.56
1:E:349:CYS:O	1:E:497:GLN:HG2	2.05	0.56
1:A:259:ARG:HB3	1:A:633:GLN:CD	2.31	0.56
1:E:217:ARG:CB	1:E:240:LEU:HD21	2.33	0.56
1:F:280:SER:O	1:F:284:LEU:HD13	2.05	0.56
1:F:474:LEU:HG	1:F:475:PRO:HD2	1.88	0.56
1:B:212:SER:HB3	1:B:238:GLU:O	2.06	0.56
1:D:428:TYR:O	1:D:429:GLN:HB2	2.05	0.56
1:A:35:LEU:C	1:A:35:LEU:HD23	2.30	0.56
1:B:351:VAL:HG22	1:B:498:VAL:HB	1.88	0.56
1:B:357:ASP:O	1:B:361:GLN:HB2	2.05	0.56
1:F:579:ASN:HB3	1:F:605:VAL:CG2	2.35	0.56
1:B:207:LEU:C	1:B:207:LEU:HD12	2.31	0.56
1:D:177:LEU:O	1:D:209:THR:HG23	2.06	0.56
1:D:364:ILE:HG23	1:D:398:ILE:HB	1.88	0.56
1:E:277:ALA:HB1	1:E:415:VAL:HG12	1.88	0.56
1:A:236:LYS:HG2	1:A:237:ARG:N	2.21	0.56
1:F:491:GLU:O	1:F:494:GLU:HB3	2.06	0.56
1:C:616:GLY:O	2:C:901:FAD:H2'	2.05	0.55
1:D:170:GLN:O	1:D:202:ARG:HB3	2.05	0.55
1:F:217:ARG:O	1:F:221:GLN:HG3	2.06	0.55
1:B:590:TYR:HB2	1:B:659:LEU:HD23	1.87	0.55
1:C:177:LEU:HB3	1:C:209:THR:HB	1.87	0.55
1:C:596:GLN:O	1:C:596:GLN:HG2	2.07	0.55
1:D:4:TYR:HD2	1:D:5:SER:N	2.05	0.55
1:D:207:LEU:C	1:D:207:LEU:HD12	2.30	0.55
1:A:64:GLU:HG3	1:A:176:PHE:HB2	1.87	0.55
1:A:463:HIS:HA	1:A:568:CYS:HB2	1.89	0.55
1:B:428:TYR:O	1:B:429:GLN:HB2	2.05	0.55
1:D:658:LYS:HZ2	1:D:659:LEU:HD13	1.72	0.55
1:F:443:LEU:HA	1:F:452:ALA:O	2.07	0.55
1:C:207:LEU:HD12	1:C:207:LEU:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:THR:O	1:D:335:ARG:HB2	2.06	0.55
1:E:655:TRP:HA	1:E:658:LYS:HE3	1.88	0.55
1:F:550:GLN:HG2	1:F:551:TRP:CE3	2.40	0.55
1:E:535:GLN:HG3	1:E:557:VAL:HG11	1.87	0.55
1:A:184:LYS:O	1:A:184:LYS:HG3	2.06	0.55
1:C:381:GLU:HA	1:C:396:SER:HB2	1.89	0.55
1:F:206:THR:HG22	1:F:243:VAL:HB	1.89	0.55
1:F:225:PHE:HB3	1:F:227:MET:HE3	1.89	0.55
1:F:284:LEU:HD23	1:F:422:GLN:CB	2.36	0.55
1:B:133:MET:HE2	1:B:375:GLU:HB2	1.88	0.55
1:B:650:ASN:O	1:B:653:ARG:HG3	2.06	0.55
1:C:456:VAL:HG22	1:C:608:ASP:HB3	1.89	0.55
1:E:570:THR:HG23	1:E:614:ALA:HB1	1.88	0.55
1:F:97:PHE:HE2	1:F:99:SER:HB2	1.72	0.55
1:E:259:ARG:HB3	1:E:633:GLN:CD	2.31	0.55
1:F:146:GLY:HA3	1:F:285:ARG:HD2	1.89	0.55
1:A:314:LEU:HD13	1:A:618:ARG:HH21	1.72	0.55
1:D:356:TRP:H	1:D:356:TRP:CD1	2.24	0.55
1:D:530:TYR:C	1:D:530:TYR:CD2	2.84	0.55
1:C:336:PHE:O	1:C:339:GLN:HG3	2.08	0.54
1:F:508:GLN:HB3	1:F:515:HIS:CD2	2.42	0.54
1:A:616:GLY:O	2:A:901:FAD:H2'	2.07	0.54
1:E:611:MET:HE2	1:E:651:PRO:HB3	1.88	0.54
1:B:435:LEU:CD1	1:B:444:LEU:HD22	2.36	0.54
1:D:334:ARG:HH11	1:D:334:ARG:CG	1.94	0.54
1:C:492:LEU:O	1:C:493:ALA:CB	2.55	0.54
1:C:572:ASP:O	1:C:573:HIS:HB2	2.07	0.54
1:D:410:GLU:HG2	1:D:414:ASN:ND2	2.23	0.54
1:E:590:TYR:OH	1:E:602:SER:O	2.24	0.54
1:F:106:THR:O	1:F:106:THR:HG22	2.07	0.54
1:F:479:VAL:HG22	1:F:523:ARG:HA	1.89	0.54
1:D:22:ARG:O	1:D:23:ASP:C	2.49	0.54
1:D:334:ARG:NH1	1:D:402:GLN:HB3	2.21	0.54
1:E:368:LEU:HD22	1:E:379:ALA:HB2	1.90	0.54
1:F:157:ILE:O	1:F:161:THR:HG23	2.08	0.54
1:F:276:SER:O	1:F:280:SER:CB	2.55	0.54
1:F:432:LEU:HD11	1:F:434:ASN:O	2.08	0.54
1:F:435:LEU:HD11	1:F:469:SER:OG	2.08	0.54
1:D:12:GLU:HB2	1:D:20:VAL:HG11	1.89	0.54
1:E:367:MET:O	1:E:370:MET:HG2	2.08	0.54
1:D:71:LEU:HD13	1:D:117:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:VAL:HG21	1:E:388:ILE:HD12	1.89	0.54
1:F:132:PRO:HD3	1:F:141:LEU:HD11	1.90	0.54
1:E:59:LEU:HD12	1:E:94:ARG:O	2.08	0.54
1:F:39:ARG:O	1:F:43:LEU:HB2	2.08	0.54
1:F:272:GLY:H	1:F:276:SER:CB	2.21	0.54
1:F:499:LEU:HD12	1:F:505:LEU:HD23	1.90	0.54
1:D:24:PHE:HD1	1:D:185:ASN:HB2	1.72	0.53
1:E:35:LEU:O	1:E:39:ARG:HG3	2.08	0.53
1:E:508:GLN:HB3	1:E:515:HIS:NE2	2.23	0.53
1:F:641:MET:HG3	1:F:645:THR:HG23	1.90	0.53
1:D:243:VAL:HG12	1:D:245:GLU:HG2	1.90	0.53
1:D:576:MET:HE2	1:D:651:PRO:HA	1.89	0.53
1:C:349:CYS:HB2	1:C:496:LYS:O	2.08	0.53
1:C:78:GLN:HG3	1:C:123:TRP:CH2	2.43	0.53
1:E:217:ARG:O	1:E:221:GLN:HG3	2.08	0.53
1:E:655:TRP:O	1:E:658:LYS:HG2	2.08	0.53
1:F:435:LEU:HD23	1:F:468:PHE:HB3	1.91	0.53
1:A:197:MET:HE2	1:A:207:LEU:HD22	1.90	0.53
1:B:315:LEU:HB2	1:B:367:MET:HE3	1.91	0.53
1:B:517:ILE:CG1	1:B:518:GLY:H	2.18	0.53
1:A:36:GLU:H	1:A:36:GLU:CD	2.16	0.53
1:B:215:PHE:HB2	1:D:249:PRO:O	2.09	0.53
1:C:584:GLU:HG3	1:F:383:ASN:HB2	1.91	0.53
1:D:14:ASN:HD21	1:D:18:THR:HG23	1.74	0.53
1:B:367:MET:O	1:B:370:MET:HG2	2.09	0.53
1:E:393:THR:OG1	1:E:546:PHE:CE1	2.61	0.53
1:F:260:THR:H	1:F:579:ASN:HD21	1.56	0.53
1:C:358:GLU:HG2	1:C:359:LYS:H	1.72	0.53
1:F:435:LEU:HD22	1:F:470:GLN:OE1	2.09	0.53
1:B:349:CYS:O	1:B:497:GLN:HG2	2.08	0.52
1:F:267:ALA:HB2	1:F:288:TRP:HZ3	1.74	0.52
1:D:583:TYR:CZ	1:D:587:LEU:HD11	2.44	0.52
1:E:601:VAL:HG12	1:E:601:VAL:O	2.09	0.52
1:A:342:VAL:HG12	1:A:344:PHE:HD1	1.75	0.52
1:A:349:CYS:O	1:A:497:GLN:HG2	2.09	0.52
1:C:232:GLY:N	1:C:238:GLU:HA	2.24	0.52
1:C:362:HIS:O	1:C:365:ALA:HB3	2.09	0.52
1:F:56:PRO:O	1:F:57:HIS:CG	2.62	0.52
1:F:237:ARG:HD2	1:F:237:ARG:N	2.24	0.52
1:B:362:HIS:O	1:B:365:ALA:HB3	2.10	0.52
1:C:519:ALA:HB3	1:C:538:ASN:CG	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LEU:HD13	1:B:117:TRP:CH2	2.45	0.52
1:D:130:GLN:HB3	1:D:141:LEU:HD13	1.92	0.52
1:D:486:ILE:CG1	1:D:515:HIS:HB2	2.39	0.52
1:E:111:ALA:O	1:E:115:GLN:HG3	2.10	0.52
1:C:523:ARG:HH22	1:C:571:ARG:HH22	1.56	0.52
1:C:285:ARG:NH2	1:C:628:GLU:OE2	2.42	0.52
1:C:290:VAL:O	1:C:424:LEU:HD12	2.10	0.52
1:D:140:ARG:C	1:D:141:LEU:HD23	2.35	0.52
1:E:207:LEU:HD11	1:E:227:MET:HE1	1.92	0.52
1:E:221:GLN:HG2	1:E:227:MET:HG2	1.92	0.52
1:E:444:LEU:HD21	1:E:457:VAL:HG21	1.91	0.52
1:F:377:ALA:HB1	1:F:398:ILE:HD11	1.92	0.52
1:F:463:HIS:HA	1:F:568:CYS:HB2	1.91	0.52
1:B:207:LEU:HD21	1:B:220:LEU:HD13	1.92	0.52
1:C:168:LEU:HG	1:C:200:LEU:HD13	1.91	0.52
1:D:217:ARG:HB2	1:D:240:LEU:HD11	1.92	0.52
1:F:353:GLN:HA	1:F:500:CYS:HB2	1.92	0.52
1:F:489:THR:HB	1:F:490:PRO:HD2	1.92	0.52
1:F:492:LEU:C	1:F:494:GLU:H	2.17	0.52
1:A:122:PRO:HG2	1:A:123:TRP:CE3	2.44	0.51
1:B:121:ALA:O	1:B:125:GLU:HG3	2.10	0.51
1:B:492:LEU:O	1:B:493:ALA:CB	2.58	0.51
1:B:648:ALA:O	1:B:653:ARG:HD3	2.10	0.51
1:D:368:LEU:CD1	1:D:379:ALA:HB2	2.40	0.51
1:C:583:TYR:CZ	1:C:587:LEU:HD11	2.45	0.51
1:C:620:LEU:HG	2:C:901:FAD:O2	2.10	0.51
1:D:517:ILE:HG12	1:D:518:GLY:N	2.21	0.51
1:E:97:PHE:CE2	1:E:99:SER:HB2	2.46	0.51
1:A:156:ASP:HB3	1:A:159:GLU:HB2	1.93	0.51
1:D:182:PRO:O	1:D:186:PRO:HB3	2.11	0.51
1:E:191:GLN:HG3	1:E:195:ASN:HD21	1.74	0.51
1:E:255:PRO:HB2	1:E:602:SER:HA	1.92	0.51
1:B:620:LEU:HB2	2:B:901:FAD:O2	2.09	0.51
1:C:286:ARG:HD3	1:C:637:GLU:OE1	2.10	0.51
1:C:620:LEU:HG	2:C:901:FAD:C2	2.40	0.51
1:D:20:VAL:HG13	1:D:21:SER:N	2.25	0.51
1:F:221:GLN:HG2	1:F:227:MET:HG3	1.93	0.51
1:F:269:ILE:O	1:F:292:LEU:HD12	2.10	0.51
1:C:299:PRO:HD3	1:C:428:TYR:CZ	2.46	0.51
1:D:343:LYS:O	1:D:414:ASN:ND2	2.42	0.51
1:D:484:SER:HB2	1:D:517:ILE:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LEU:HD23	1:A:348:TRP:CZ3	2.46	0.51
1:A:322:LEU:HA	1:A:574:LEU:HD21	1.93	0.51
1:F:530:TYR:HE2	1:F:532:GLU:HG3	1.74	0.51
1:D:385:VAL:HG12	1:D:391:VAL:O	2.10	0.51
1:E:97:PHE:HE2	1:E:99:SER:HB2	1.75	0.51
1:F:284:LEU:HD11	1:F:290:VAL:HB	1.93	0.51
1:A:315:LEU:HD12	1:A:367:MET:HE3	1.93	0.51
1:F:405:TRP:CD1	1:F:507:PRO:HD2	2.45	0.51
1:B:256:TRP:CD1	1:B:656:VAL:HG11	2.46	0.51
1:E:121:ALA:N	1:E:122:PRO:HD2	2.26	0.51
1:F:275:ALA:O	1:F:279:LEU:HB2	2.11	0.51
1:A:211:THR:O	1:A:240:LEU:HB2	2.11	0.51
1:C:320:GLU:O	1:C:321:ALA:HB3	2.11	0.51
1:C:504:TYR:CE2	1:C:518:GLY:HA3	2.46	0.51
1:F:278:LEU:HD12	1:F:623:ALA:HB1	1.93	0.51
1:B:177:LEU:O	1:B:209:THR:HG23	2.10	0.50
1:C:657:ARG:O	1:C:657:ARG:HD3	2.10	0.50
1:D:518:GLY:HA3	1:D:538:ASN:ND2	2.26	0.50
1:F:122:PRO:HG2	1:F:123:TRP:CE3	2.46	0.50
1:F:267:ALA:HB2	1:F:288:TRP:CZ3	2.45	0.50
1:F:463:HIS:NE2	1:F:464:GLN:HG3	2.26	0.50
1:A:523:ARG:HG2	1:A:523:ARG:HH11	1.76	0.50
1:E:269:ILE:HG12	1:E:458:VAL:HG13	1.93	0.50
1:E:508:GLN:O	1:E:510:PRO:HD3	2.11	0.50
1:B:342:VAL:HG13	1:B:414:ASN:HB3	1.92	0.50
1:A:170:GLN:O	1:A:202:ARG:HB3	2.12	0.50
1:E:515:HIS:N	1:E:515:HIS:CD2	2.80	0.50
1:F:40:TYR:HE1	1:F:230:ARG:NH1	2.09	0.50
1:F:380:VAL:HG21	1:F:399:THR:OG1	2.10	0.50
1:F:435:LEU:HD21	1:F:468:PHE:HB3	1.93	0.50
1:C:458:VAL:HG22	1:C:610:PHE:HB2	1.94	0.50
1:D:29:PHE:CG	1:D:117:TRP:HH2	2.30	0.50
1:E:383:ASN:OD1	1:E:383:ASN:N	2.44	0.50
1:F:280:SER:OG	1:F:424:LEU:HD22	2.10	0.50
1:A:286:ARG:HG3	1:A:286:ARG:HH11	1.76	0.50
1:D:41:VAL:HG22	1:D:239:MET:HE1	1.93	0.50
1:E:217:ARG:HB2	1:E:240:LEU:CD2	2.37	0.50
1:E:372:LEU:H	1:E:372:LEU:HD12	1.76	0.50
1:B:39:ARG:O	1:B:43:LEU:HB2	2.11	0.50
1:D:98:ILE:CD1	1:D:168:LEU:HD11	2.42	0.50
1:D:104:PRO:HG3	1:D:154:PHE:CD1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:389:THR:O	1:D:495:LEU:HD12	2.11	0.50
1:F:114:HIS:ND1	1:F:115:GLN:HG3	2.27	0.50
1:A:518:GLY:O	1:A:519:ALA:CB	2.59	0.50
1:D:485:HIS:CE1	1:D:563:ARG:HG2	2.47	0.50
1:D:517:ILE:HD12	1:D:555:VAL:HG11	1.92	0.50
1:F:131:TRP:CD2	1:F:132:PRO:HD2	2.47	0.50
1:A:121:ALA:N	1:A:122:PRO:HD2	2.27	0.49
1:A:596:GLN:HA	1:A:596:GLN:HE21	1.76	0.49
1:B:110:LEU:HG	1:B:114:HIS:CE1	2.47	0.49
1:C:354:LEU:HD23	1:C:546:PHE:HZ	1.77	0.49
1:D:435:LEU:HB3	1:D:444:LEU:HD23	1.94	0.49
1:F:325:PHE:O	1:F:329:ALA:CB	2.60	0.49
1:C:97:PHE:O	1:C:150:LEU:HD12	2.12	0.49
1:C:418:LEU:HD11	1:C:422:GLN:HE21	1.77	0.49
1:D:485:HIS:NE2	1:D:563:ARG:HG2	2.26	0.49
1:E:177:LEU:O	1:E:209:THR:HG23	2.12	0.49
1:E:577:VAL:HA	1:E:611:MET:O	2.12	0.49
1:B:122:PRO:HG2	1:B:123:TRP:CZ3	2.48	0.49
1:B:461:ASN:HB2	2:B:901:FAD:C8A	2.42	0.49
1:B:518:GLY:CA	1:B:538:ASN:CG	2.84	0.49
1:D:435:LEU:HD12	1:D:435:LEU:H	1.77	0.49
1:E:236:LYS:HD3	1:E:237:ARG:N	2.27	0.49
1:B:303:ALA:HB1	2:B:901:FAD:H3'	1.93	0.49
1:B:391:VAL:HG11	1:B:551:TRP:CZ2	2.48	0.49
1:C:112:LEU:O	1:C:115:GLN:HB2	2.12	0.49
1:C:583:TYR:CE2	1:C:587:LEU:HD11	2.47	0.49
1:E:340:LEU:HD12	1:E:341:PRO:HD2	1.94	0.49
1:F:105:LEU:O	1:F:109:ASP:OD1	2.30	0.49
1:A:593:LEU:O	1:A:594:ALA:C	2.55	0.49
1:C:625:LEU:O	1:C:629:ILE:HG13	2.12	0.49
1:D:56:PRO:O	1:D:57:HIS:CG	2.66	0.49
1:D:184:LYS:O	1:D:185:ASN:HB3	2.11	0.49
1:E:274:ILE:HG23	1:E:275:ALA:N	2.27	0.49
1:E:484:SER:CB	1:E:538:ASN:HD22	2.26	0.49
1:E:517:ILE:HG23	1:E:518:GLY:N	2.26	0.49
1:C:467:ARG:O	1:F:374:ALA:HB1	2.12	0.49
1:D:50:VAL:O	1:D:53:PRO:HG2	2.12	0.49
1:F:474:LEU:HD21	1:F:611:MET:HE1	1.94	0.49
1:F:602:SER:OG	1:F:604:PRO:HD3	2.13	0.49
1:E:66:GLY:HA2	1:E:100:PHE:O	2.12	0.49
1:E:315:LEU:HD13	1:E:372:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:483:VAL:HG21	1:E:504:TYR:OH	2.12	0.49
1:F:435:LEU:HD13	1:F:470:GLN:NE2	2.27	0.49
1:F:579:ASN:HB3	1:F:605:VAL:HG13	1.95	0.49
1:A:280:SER:O	1:A:284:LEU:HG	2.12	0.49
1:C:133:MET:HE1	1:C:376:LEU:HA	1.94	0.49
1:B:504:TYR:CE2	1:B:519:ALA:HB2	2.48	0.49
1:C:584:GLU:CD	1:F:381:GLU:HB3	2.37	0.49
1:D:492:LEU:O	1:D:493:ALA:CB	2.60	0.49
1:E:486:ILE:HD13	1:E:555:VAL:HG13	1.94	0.49
1:F:105:LEU:O	1:F:105:LEU:HG	2.12	0.49
1:D:110:LEU:HD22	1:D:131:TRP:CD2	2.48	0.48
1:D:259:ARG:NH2	1:D:646:LEU:O	2.45	0.48
1:D:484:SER:HB2	1:D:517:ILE:CG2	2.43	0.48
1:E:324:ARG:NH1	1:E:324:ARG:CG	2.64	0.48
1:C:121:ALA:N	1:C:122:PRO:HD2	2.28	0.48
1:C:545:CYS:C	1:C:547:PRO:HD3	2.38	0.48
1:D:10:ASN:N	1:D:10:ASN:HD22	2.11	0.48
1:E:539:ARG:HG2	1:E:543:ILE:HD13	1.94	0.48
1:E:102:LYS:HA	1:E:155:GLY:O	2.13	0.48
1:F:307:ARG:HB2	1:F:485:HIS:CE1	2.44	0.48
1:A:334:ARG:NH1	1:A:338:ASP:OD2	2.46	0.48
1:A:474:LEU:HD13	1:A:611:MET:HE1	1.95	0.48
1:C:408:PRO:HB3	1:C:620:LEU:HD21	1.95	0.48
1:F:134:PRO:HA	1:F:154:PHE:CE2	2.47	0.48
1:F:303:ALA:N	2:F:901:FAD:O2A	2.46	0.48
1:F:623:ALA:HB3	1:F:624:PRO:HD3	1.95	0.48
1:A:111:ALA:HA	1:A:128:GLN:NE2	2.28	0.48
1:A:305:GLY:O	1:A:563:ARG:HD2	2.14	0.48
1:B:285:ARG:HH22	1:B:286:ARG:NH2	2.11	0.48
1:C:35:LEU:HD22	1:C:39:ARG:NH2	2.27	0.48
1:D:270:ILE:HG12	1:D:432:LEU:HD22	1.94	0.48
1:E:165:ASP:HA	1:E:643:ALA:HB2	1.94	0.48
1:F:172:VAL:HB	1:F:200:LEU:O	2.14	0.48
1:F:313:PRO:HD3	1:F:330:PHE:CD1	2.49	0.48
1:A:595:GLU:HA	1:E:477:TYR:CB	2.27	0.48
1:C:37:GLU:HB2	1:C:233:PHE:CZ	2.47	0.48
4:C:693:HOH:O	1:F:102:LYS:HE3	2.12	0.48
1:D:370:MET:HG3	1:D:372:LEU:HD21	1.94	0.48
1:F:144:ASP:C	1:F:145:GLU:HG2	2.39	0.48
1:A:349:CYS:HB2	1:A:496:LYS:O	2.13	0.48
1:B:575:PRO:O	1:B:653:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LEU:HD12	1:D:208:ALA:N	2.28	0.48
1:E:596:GLN:HG2	1:E:599:GLU:HG2	1.95	0.48
1:F:197:MET:O	1:F:201:ALA:HB2	2.12	0.48
1:F:299:PRO:HG2	1:F:413:ARG:HG3	1.95	0.48
1:F:355:GLY:H	1:F:364:ILE:HD12	1.78	0.48
1:C:138:CYS:HB2	1:C:153:TRP:CE2	2.48	0.48
1:C:207:LEU:C	1:C:207:LEU:CD1	2.86	0.48
1:C:572:ASP:CG	1:C:653:ARG:NH1	2.71	0.48
1:E:612:PHE:CE2	1:E:615:LEU:HD21	2.45	0.48
1:F:86:ALA:HB3	1:F:87:HIS:HD2	1.78	0.48
1:F:486:ILE:HD12	1:F:555:VAL:HG22	1.95	0.48
1:A:406:LEU:HG	1:A:620:LEU:HD13	1.96	0.48
1:B:230:ARG:NH2	1:B:239:MET:HE1	2.29	0.48
1:C:329:ALA:HA	1:C:625:LEU:HD22	1.96	0.48
1:E:322:LEU:HA	1:E:574:LEU:HD21	1.96	0.48
1:E:557:VAL:HG12	1:E:557:VAL:O	2.13	0.48
1:F:340:LEU:HD12	1:F:341:PRO:HD2	1.96	0.48
1:F:367:MET:O	1:F:370:MET:HG3	2.14	0.48
1:F:642:ASP:CG	1:F:645:THR:HG22	2.39	0.48
1:A:501:TYR:N	1:A:501:TYR:CD2	2.82	0.48
1:E:394:ASN:O	1:E:394:ASN:CG	2.57	0.48
1:E:535:GLN:HG3	1:E:557:VAL:HG12	1.96	0.48
1:F:292:LEU:HB3	1:F:426:ILE:HG12	1.95	0.48
1:F:501:TYR:OH	1:F:517:ILE:HG13	2.13	0.48
1:C:110:LEU:HD22	1:C:131:TRP:CD2	2.49	0.47
1:D:3:HIS:O	1:D:3:HIS:CD2	2.67	0.47
1:D:24:PHE:CD1	1:D:185:ASN:HB2	2.49	0.47
1:D:355:GLY:HA3	1:D:361:GLN:HG3	1.96	0.47
1:E:484:SER:OG	1:E:538:ASN:ND2	2.47	0.47
1:F:250:LEU:HD12	1:F:250:LEU:H	1.79	0.47
1:F:463:HIS:CD2	1:F:464:GLN:HG3	2.49	0.47
1:F:579:ASN:HB3	1:F:605:VAL:HG22	1.96	0.47
1:F:642:ASP:OD2	1:F:645:THR:HG22	2.14	0.47
1:C:43:LEU:HB3	1:C:49:GLU:OE2	2.14	0.47
1:C:428:TYR:O	1:C:429:GLN:HB2	2.14	0.47
1:C:505:LEU:HD12	1:C:506:THR:H	1.79	0.47
1:D:410:GLU:HG2	1:D:414:ASN:HD21	1.78	0.47
1:E:144:ASP:O	1:E:145:GLU:HG2	2.14	0.47
1:E:180:PHE:HB2	1:E:185:ASN:HB3	1.95	0.47
1:F:443:LEU:HD22	1:F:452:ALA:O	2.13	0.47
1:D:181:ALA:O	1:D:183:ALA:O	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:550:GLN:HG2	1:D:551:TRP:H	1.78	0.47
1:E:399:THR:O	1:E:401:PRO:HD3	2.14	0.47
1:A:314:LEU:HD13	1:A:618:ARG:NH2	2.28	0.47
1:B:121:ALA:N	1:B:122:PRO:HD2	2.29	0.47
1:B:485:HIS:HE1	4:B:674:HOH:O	1.97	0.47
1:C:130:GLN:HB3	1:C:141:LEU:HD13	1.97	0.47
1:C:271:GLY:CA	1:C:292:LEU:HD11	2.29	0.47
1:A:207:LEU:HD21	1:A:220:LEU:HD22	1.97	0.47
1:E:391:VAL:HG22	1:E:551:TRP:CD1	2.50	0.47
1:E:518:GLY:CA	1:E:538:ASN:CG	2.87	0.47
1:F:133:MET:HE2	1:F:375:GLU:HB3	1.97	0.47
1:C:342:VAL:HG13	1:C:414:ASN:HB3	1.96	0.47
1:C:411:LEU:O	1:C:415:VAL:HG23	2.15	0.47
2:C:901:FAD:H9	2:C:901:FAD:H1'2	1.71	0.47
1:C:181:ALA:O	1:C:183:ALA:O	2.33	0.47
1:C:501:TYR:CD1	1:C:503:GLY:N	2.82	0.47
1:D:259:ARG:NH1	1:D:577:VAL:O	2.47	0.47
1:E:168:LEU:HG	1:E:200:LEU:HD22	1.97	0.47
1:E:299:PRO:HD3	1:E:428:TYR:CE2	2.50	0.47
1:B:78:GLN:HG3	1:B:123:TRP:CH2	2.49	0.47
1:B:380:VAL:HG22	1:B:384:ALA:HB1	1.97	0.47
1:C:602:SER:O	1:C:603:ALA:C	2.58	0.47
1:D:248:LEU:HA	1:D:249:PRO:HD3	1.75	0.47
1:A:175:TRP:HB2	1:A:207:LEU:CB	2.45	0.47
1:B:170:GLN:O	1:B:202:ARG:HD3	2.15	0.47
1:C:271:GLY:O	2:C:901:FAD:H1B	2.15	0.47
1:E:439:ASP:CG	1:E:440:ASP:H	2.23	0.47
1:F:256:TRP:HB2	1:F:656:VAL:HG11	1.96	0.46
1:B:39:ARG:HA	1:B:43:LEU:HD22	1.95	0.46
1:D:356:TRP:CD2	1:D:357:ASP:HB2	2.49	0.46
1:F:256:TRP:CH2	1:F:597:LYS:HB3	2.51	0.46
1:D:317:LYS:HE3	1:D:318:HIS:HE1	1.81	0.46
1:E:275:ALA:HB2	1:E:615:LEU:HD11	1.96	0.46
1:B:356:TRP:CZ2	1:B:502:ASP:HB2	2.50	0.46
1:B:590:TYR:CB	1:B:659:LEU:HD23	2.44	0.46
1:B:642:ASP:OD1	1:B:645:THR:HG23	2.16	0.46
1:D:514:HIS:C	1:D:515:HIS:HD2	2.23	0.46
1:E:488:THR:HG22	1:E:513:GLN:O	2.14	0.46
1:F:343:LYS:HE2	1:F:414:ASN:HD21	1.81	0.46
1:F:40:TYR:HE1	1:F:230:ARG:HH12	1.64	0.46
1:B:545:CYS:C	1:B:547:PRO:HD3	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ILE:O	1:C:292:LEU:HD12	2.16	0.46
1:A:307:ARG:NH2	1:A:485:HIS:HB3	2.30	0.46
1:C:306:ASN:HB2	4:C:680:HOH:O	2.16	0.46
1:F:110:LEU:HD21	1:F:127:LEU:HG	1.96	0.46
1:F:112:LEU:C	1:F:114:HIS:N	2.73	0.46
1:F:486:ILE:HG13	1:F:515:HIS:HB2	1.96	0.46
1:F:489:THR:HB	1:F:490:PRO:CD	2.46	0.46
1:F:603:ALA:N	1:F:604:PRO:HD3	2.31	0.46
1:A:66:GLY:HA2	1:A:100:PHE:O	2.16	0.46
1:A:175:TRP:HB2	1:A:207:LEU:HB3	1.96	0.46
1:B:64:GLU:OE2	1:B:72:ASN:HB2	2.15	0.46
1:B:177:LEU:CB	1:B:209:THR:HG23	2.40	0.46
1:C:357:ASP:O	1:C:361:GLN:HB2	2.16	0.46
1:C:390:GLY:HA3	1:C:494:GLU:O	2.16	0.46
1:D:353:GLN:HG2	1:D:398:ILE:CG2	2.45	0.46
1:E:461:ASN:HB2	2:E:901:FAD:C8A	2.45	0.46
1:F:399:THR:O	1:F:401:PRO:HD3	2.15	0.46
1:A:359:LYS:O	1:A:363:LYS:HG2	2.16	0.46
1:A:619:GLY:HA3	2:A:901:FAD:O2'	2.15	0.46
1:C:61:VAL:HG22	1:C:96:HIS:HB3	1.98	0.46
1:D:41:VAL:HG22	1:D:239:MET:CE	2.45	0.46
1:D:307:ARG:HG3	1:D:485:HIS:CE1	2.51	0.46
1:D:357:ASP:CG	1:D:358:GLU:N	2.74	0.46
1:E:83:PHE:CE2	1:E:92:LEU:HD23	2.51	0.46
1:B:391:VAL:CG1	1:B:551:TRP:CZ2	2.99	0.46
1:C:416:LEU:O	1:C:420:GLN:HG3	2.15	0.46
1:C:463:HIS:HA	1:C:568:CYS:HB2	1.98	0.46
1:F:121:ALA:N	1:F:122:PRO:HD2	2.30	0.46
1:B:37:GLU:HG3	1:B:233:PHE:CD2	2.51	0.45
1:B:71:LEU:HD13	1:B:117:TRP:CZ2	2.50	0.45
1:B:340:LEU:HD12	1:B:341:PRO:HD2	1.97	0.45
1:D:29:PHE:CD2	1:D:117:TRP:CH2	3.04	0.45
1:D:65:SER:HB2	1:D:188:MET:HE3	1.97	0.45
1:D:430:TYR:HB3	1:D:446:PHE:CD1	2.50	0.45
1:E:256:TRP:O	1:E:603:ALA:HB2	2.16	0.45
1:E:256:TRP:CD1	1:E:656:VAL:HG11	2.51	0.45
1:F:277:ALA:HB1	1:F:415:VAL:HG12	1.98	0.45
1:A:232:GLY:HA3	1:A:237:ARG:O	2.17	0.45
1:A:571:ARG:O	1:A:572:ASP:OD1	2.35	0.45
1:B:177:LEU:O	1:B:209:THR:CG2	2.65	0.45
1:B:229:LYS:HD3	1:B:238:GLU:OE2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:GLU:CB	1:C:176:PHE:HB2	2.46	0.45
1:D:52:PHE:N	1:D:53:PRO:HD2	2.31	0.45
1:D:349:CYS:HB2	1:D:496:LYS:O	2.16	0.45
1:F:64:GLU:HG2	1:F:66:GLY:O	2.17	0.45
1:F:255:PRO:O	1:F:258:ASN:HB2	2.16	0.45
1:A:104:PRO:C	1:A:105:LEU:HD12	2.41	0.45
1:A:220:LEU:HD13	1:A:227:MET:HE2	1.97	0.45
1:A:428:TYR:O	1:A:429:GLN:HB2	2.16	0.45
1:D:504:TYR:HE2	1:D:519:ALA:HB2	1.81	0.45
1:E:480:ALA:HB2	1:E:525:SER:O	2.17	0.45
1:E:517:ILE:HG23	1:E:538:ASN:HB3	1.98	0.45
1:F:114:HIS:CD2	1:F:121:ALA:HB1	2.51	0.45
1:B:237:ARG:HH21	1:D:599:GLU:HG2	1.81	0.45
1:C:618:ARG:HG3	1:C:618:ARG:NH1	2.26	0.45
1:D:13:PHE:O	1:D:14:ASN:CB	2.65	0.45
1:D:479:VAL:O	1:D:567:ARG:HG2	2.16	0.45
1:E:41:VAL:HA	1:E:239:MET:HE1	1.99	0.45
1:E:446:PHE:HB2	1:E:450:GLN:HB2	1.99	0.45
1:F:367:MET:HE1	1:F:400:TYR:OH	2.17	0.45
1:A:593:LEU:HD12	1:A:593:LEU:HA	1.74	0.45
1:B:368:LEU:HD13	1:B:379:ALA:HB2	1.99	0.45
1:C:42:PHE:CZ	1:C:178:ASP:HB2	2.52	0.45
1:C:356:TRP:CD1	1:C:356:TRP:H	2.33	0.45
1:C:586:THR:HA	1:C:604:PRO:HG2	1.98	0.45
1:D:437:ARG:HD2	1:D:441:CYS:O	2.17	0.45
1:D:489:THR:HB	1:D:490:PRO:CD	2.44	0.45
1:E:78:GLN:HG3	1:E:123:TRP:CH2	2.51	0.45
1:B:164:LEU:HD13	1:B:200:LEU:HD11	1.99	0.45
1:E:191:GLN:HG3	1:E:195:ASN:ND2	2.31	0.45
1:E:518:GLY:HA3	1:E:538:ASN:ND2	2.32	0.45
1:E:596:GLN:CG	1:E:599:GLU:HG2	2.47	0.45
1:F:356:TRP:CD1	1:F:356:TRP:N	2.85	0.45
1:F:432:LEU:HD13	1:F:444:LEU:HB3	1.99	0.45
1:A:67:PHE:O	1:A:68:GLY:C	2.60	0.45
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.17	0.45
1:B:258:ASN:HD22	1:B:602:SER:HB2	1.82	0.45
1:B:355:GLY:HA2	1:B:360:SER:HB2	1.98	0.45
1:C:568:CYS:O	1:C:614:ALA:HA	2.16	0.45
1:D:384:ALA:O	1:D:387:GLN:HG2	2.17	0.45
1:E:183:ALA:O	1:E:184:LYS:HB2	2.16	0.45
1:B:159:GLU:OE2	1:D:190:THR:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PRO:HG2	1:C:123:TRP:CE3	2.52	0.45
1:D:501:TYR:CE2	1:D:542:LEU:HD13	2.52	0.45
1:F:473:THR:HG21	1:F:583:TYR:CD2	2.52	0.45
1:F:473:THR:HG21	1:F:583:TYR:HD2	1.82	0.45
1:C:437:ARG:HH11	1:C:442:TRP:CD1	2.34	0.45
1:D:9:ALA:O	1:D:10:ASN:CB	2.65	0.45
1:D:655:TRP:O	1:D:659:LEU:HB2	2.16	0.45
1:F:133:MET:HA	1:F:134:PRO:HD3	1.78	0.45
1:A:372:LEU:HB3	1:A:373:PRO:HD2	1.99	0.44
1:C:375:GLU:O	1:C:401:PRO:HG2	2.16	0.44
1:D:11:LEU:HD11	1:D:20:VAL:O	2.17	0.44
1:D:308:GLN:NE2	1:D:509:ASN:HB2	2.33	0.44
1:E:269:ILE:HG12	1:E:458:VAL:CG1	2.47	0.44
1:E:648:ALA:O	1:E:653:ARG:HD3	2.17	0.44
1:F:221:GLN:CG	1:F:227:MET:HG3	2.47	0.44
1:F:605:VAL:O	1:F:606:PHE:C	2.59	0.44
1:E:430:TYR:HD1	1:E:446:PHE:CD2	2.34	0.44
1:F:386:GLU:HA	1:F:391:VAL:O	2.17	0.44
1:F:475:PRO:HB2	1:F:654:LEU:HD12	1.98	0.44
1:F:484:SER:HB2	1:F:517:ILE:CG2	2.47	0.44
1:F:650:ASN:O	1:F:653:ARG:HB2	2.17	0.44
1:F:650:ASN:OD1	1:F:651:PRO:HD2	2.17	0.44
1:A:550:GLN:NE2	1:A:553:LYS:CE	2.79	0.44
1:B:256:TRP:O	1:B:603:ALA:HB2	2.17	0.44
1:B:435:LEU:HD11	1:B:444:LEU:HD22	1.97	0.44
1:D:3:HIS:O	1:D:4:TYR:HB3	2.18	0.44
1:D:313:PRO:HD3	1:D:330:PHE:CZ	2.51	0.44
1:E:110:LEU:HG	1:E:114:HIS:CE1	2.53	0.44
1:F:209:THR:CG2	1:F:211:THR:HG22	2.47	0.44
1:A:86:ALA:HB3	1:A:87:HIS:CD2	2.52	0.44
1:D:458:VAL:HG22	1:D:610:PHE:HB2	1.99	0.44
1:F:370:MET:CE	1:F:372:LEU:HD11	2.47	0.44
1:F:378:VAL:HG12	1:F:399:THR:HB	1.99	0.44
1:F:576:MET:HE2	1:F:653:ARG:NH1	2.30	0.44
1:F:656:VAL:O	1:F:660:LEU:HG	2.18	0.44
1:A:408:PRO:HB3	1:A:620:LEU:HD21	1.99	0.44
1:A:595:GLU:CA	1:E:477:TYR:HB3	2.28	0.44
1:C:106:THR:O	1:C:107:ARG:C	2.59	0.44
1:D:36:GLU:HA	1:D:36:GLU:OE1	2.18	0.44
1:D:185:ASN:O	1:D:185:ASN:CG	2.60	0.44
1:E:260:THR:HB	1:E:579:ASN:ND2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:O	1:A:660:LEU:HG	2.17	0.44
1:C:584:GLU:CG	1:F:381:GLU:HB3	2.46	0.44
1:D:22:ARG:HD2	1:D:22:ARG:HA	1.84	0.44
1:E:551:TRP:O	1:E:554:GLU:HB2	2.18	0.44
1:E:596:GLN:HE21	1:E:599:GLU:HG3	1.83	0.44
1:F:274:ILE:HG13	1:F:304:SER:OG	2.17	0.44
1:A:579:ASN:H	1:A:579:ASN:HD22	1.65	0.44
1:C:170:GLN:CD	1:C:250:LEU:HD21	2.42	0.44
1:B:120:LEU:C	1:B:122:PRO:HD2	2.43	0.44
1:D:4:TYR:CD2	1:D:5:SER:N	2.85	0.44
1:E:164:LEU:HD13	1:E:168:LEU:HD23	2.00	0.44
1:E:256:TRP:HD1	1:E:656:VAL:HG11	1.83	0.44
1:E:265:ARG:HD3	1:E:265:ARG:HA	1.78	0.44
1:F:177:LEU:HD22	1:F:189:TRP:CZ3	2.53	0.44
1:F:625:LEU:O	1:F:629:ILE:HG12	2.18	0.44
1:A:286:ARG:HG3	1:A:286:ARG:NH1	2.33	0.44
1:A:381:GLU:O	1:A:385:VAL:HG23	2.18	0.44
1:A:650:ASN:HA	1:A:651:PRO:HD3	1.86	0.44
1:B:112:LEU:O	1:B:115:GLN:HB2	2.18	0.44
1:B:486:ILE:HD12	1:B:555:VAL:HG13	2.00	0.44
1:C:444:LEU:HD21	1:C:457:VAL:HG21	1.99	0.44
1:C:501:TYR:CE2	1:C:542:LEU:HD13	2.53	0.44
1:D:29:PHE:CG	1:D:117:TRP:CH2	3.06	0.44
1:D:170:GLN:HA	1:D:201:ALA:O	2.17	0.44
1:D:391:VAL:HG13	1:D:392:ALA:N	2.33	0.44
1:F:100:PHE:CG	1:F:157:ILE:HG13	2.52	0.44
1:F:199:ARG:HG3	1:F:251:PRO:HG2	1.99	0.44
1:C:406:LEU:HD12	1:C:406:LEU:C	2.43	0.43
1:C:629:ILE:HG23	1:C:639:ILE:CG2	2.48	0.43
1:D:441:CYS:HB2	1:D:454:HIS:O	2.18	0.43
1:F:576:MET:N	1:F:614:ALA:HB3	2.30	0.43
1:A:244:MET:HE2	1:A:244:MET:HB2	1.88	0.43
1:C:381:GLU:N	1:C:381:GLU:OE1	2.50	0.43
1:D:356:TRP:CE3	1:D:357:ASP:HB2	2.53	0.43
1:D:411:LEU:O	1:D:415:VAL:HG23	2.18	0.43
1:E:191:GLN:OE1	1:E:194:PHE:HD2	2.01	0.43
1:A:265:ARG:HD3	1:A:265:ARG:HA	1.80	0.43
1:A:551:TRP:O	1:A:554:GLU:HB2	2.18	0.43
1:B:250:LEU:HA	1:B:251:PRO:HD3	1.74	0.43
1:C:189:TRP:N	1:C:189:TRP:CD1	2.86	0.43
1:D:603:ALA:HA	1:D:604:PRO:HD3	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:LEU:CD2	1:E:393:THR:HG21	2.48	0.43
1:F:269:ILE:HD11	1:F:283:LEU:HD12	1.99	0.43
1:F:603:ALA:N	1:F:604:PRO:CD	2.81	0.43
1:D:530:TYR:C	1:D:530:TYR:HD2	2.26	0.43
1:E:270:ILE:HG22	1:E:461:ASN:HB3	2.00	0.43
1:F:265:ARG:HA	1:F:265:ARG:HD3	1.78	0.43
1:A:435:LEU:HD22	1:A:444:LEU:HD22	2.01	0.43
1:B:386:GLU:HA	1:B:391:VAL:O	2.18	0.43
1:C:69:THR:HG22	1:C:105:LEU:HD11	2.00	0.43
1:C:383:ASN:ND2	1:C:383:ASN:H	2.15	0.43
1:F:334:ARG:HB3	1:F:334:ARG:NH1	2.33	0.43
1:B:479:VAL:HA	1:B:522:HIS:O	2.18	0.43
1:C:352:THR:HG23	1:C:497:GLN:OE1	2.19	0.43
1:D:270:ILE:N	1:D:270:ILE:HD12	2.34	0.43
1:E:177:LEU:HB3	1:E:209:THR:OG1	2.19	0.43
1:E:642:ASP:OD1	1:E:642:ASP:C	2.62	0.43
1:F:86:ALA:CB	1:F:87:HIS:HD2	2.31	0.43
1:F:256:TRP:HH2	1:F:597:LYS:HB3	1.83	0.43
1:F:593:LEU:HD13	1:F:600:ALA:HB2	2.01	0.43
1:B:411:LEU:O	1:B:415:VAL:HG23	2.19	0.43
1:D:307:ARG:HE	1:D:563:ARG:NH2	2.16	0.43
1:D:355:GLY:HA2	1:D:360:SER:HB2	2.01	0.43
1:D:377:ALA:HA	1:D:399:THR:O	2.19	0.43
1:F:354:LEU:CD1	1:F:393:THR:HG21	2.48	0.43
2:F:901:FAD:C2'	2:F:901:FAD:N1	2.82	0.43
1:A:329:ALA:HB2	1:A:625:LEU:HD23	2.00	0.43
1:D:2:LYS:HD3	1:D:2:LYS:HA	1.82	0.43
1:D:64:GLU:HG3	1:D:178:ASP:OD1	2.19	0.43
1:D:353:GLN:CB	1:D:500:CYS:HB2	2.49	0.43
1:E:207:LEU:C	1:E:207:LEU:CD1	2.91	0.43
1:E:387:GLN:HG3	1:E:388:ILE:N	2.33	0.43
1:E:406:LEU:HD11	1:E:620:LEU:HD13	2.01	0.43
1:F:112:LEU:O	1:F:115:GLN:N	2.51	0.43
1:B:380:VAL:HG21	1:B:388:ILE:HD13	2.01	0.43
1:C:502:ASP:HB2	1:C:545:CYS:SG	2.59	0.43
1:C:570:THR:CG2	1:C:576:MET:HE3	2.48	0.43
1:E:438:LYS:HG2	1:E:439:ASP:H	1.84	0.43
1:A:391:VAL:CG1	1:A:551:TRP:CE2	3.01	0.43
1:C:138:CYS:HB2	1:C:153:TRP:CZ2	2.54	0.43
1:E:141:LEU:HD12	1:E:150:LEU:HD23	2.01	0.43
1:F:105:LEU:HB3	1:F:131:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:LEU:CD2	1:F:611:MET:HE1	2.49	0.43
1:A:274:ILE:HD13	1:A:411:LEU:HD23	2.00	0.42
1:B:108:ALA:HB1	1:C:190:THR:HG22	2.01	0.42
1:D:339:GLN:O	1:D:339:GLN:HG2	2.19	0.42
1:E:508:GLN:HB3	1:E:515:HIS:CD2	2.54	0.42
1:F:78:GLN:HG3	1:F:123:TRP:CH2	2.54	0.42
1:F:175:TRP:CH2	1:F:197:MET:HG2	2.53	0.42
1:F:581:PRO:HA	1:F:605:VAL:H	1.84	0.42
1:A:592:SER:O	1:A:593:LEU:C	2.61	0.42
1:B:43:LEU:CD1	1:B:43:LEU:N	2.82	0.42
1:B:492:LEU:C	1:B:494:GLU:H	2.27	0.42
1:C:141:LEU:HD23	1:C:141:LEU:N	2.34	0.42
1:F:106:THR:CG2	1:F:108:ALA:HB3	2.50	0.42
1:A:325:PHE:HB2	1:A:645:THR:CG2	2.49	0.42
1:A:589:GLU:O	1:A:590:TYR:HB2	2.19	0.42
1:B:271:GLY:O	2:B:901:FAD:H1B	2.18	0.42
1:C:618:ARG:HH11	1:C:618:ARG:HG2	1.79	0.42
1:D:133:MET:CE	1:D:376:LEU:HB2	2.46	0.42
1:E:272:GLY:H	1:E:276:SER:CB	2.32	0.42
1:F:103:PHE:HA	1:F:104:PRO:HD2	1.83	0.42
1:F:135:LEU:HB2	1:F:139:HIS:CE1	2.55	0.42
1:F:279:LEU:HD21	1:F:630:LEU:HB3	2.02	0.42
1:F:355:GLY:N	1:F:364:ILE:HD12	2.35	0.42
1:F:488:THR:HB	1:F:515:HIS:CD2	2.54	0.42
1:C:326:PHE:O	1:C:330:PHE:HB3	2.19	0.42
1:E:406:LEU:C	1:E:406:LEU:HD12	2.43	0.42
1:F:536:GLN:HE21	1:F:536:GLN:HB3	1.69	0.42
1:B:332:PHE:CD1	1:B:332:PHE:C	2.97	0.42
1:B:476:VAL:HG12	1:B:570:THR:HG22	2.00	0.42
1:C:619:GLY:HA3	2:C:901:FAD:O2'	2.19	0.42
1:D:391:VAL:CG1	1:D:392:ALA:N	2.80	0.42
1:F:530:TYR:C	1:F:530:TYR:CD2	2.98	0.42
1:A:43:LEU:N	1:A:43:LEU:HD12	2.34	0.42
1:B:299:PRO:HD3	1:B:428:TYR:CZ	2.54	0.42
1:B:520:SER:O	1:B:567:ARG:NH2	2.52	0.42
1:B:658:LYS:HE3	1:B:659:LEU:CD1	2.50	0.42
1:C:584:GLU:HG2	1:F:381:GLU:CB	2.50	0.42
1:D:353:GLN:HG2	1:D:398:ILE:HG22	2.01	0.42
1:E:56:PRO:HA	1:E:91:GLN:NE2	2.34	0.42
1:E:357:ASP:OD1	1:E:357:ASP:C	2.63	0.42
1:F:278:LEU:HD22	1:F:336:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:342:VAL:HG23	1:F:418:LEU:HD13	2.01	0.42
1:F:642:ASP:OD1	1:F:644:SER:HB3	2.19	0.42
1:D:269:ILE:O	1:D:292:LEU:HD12	2.20	0.42
1:D:280:SER:O	1:D:284:LEU:HG	2.20	0.42
1:E:60:PHE:HB2	1:E:92:LEU:HD11	2.02	0.42
2:F:901:FAD:H9	2:F:901:FAD:H1'1	1.71	0.42
1:A:177:LEU:HB3	1:A:209:THR:HB	2.00	0.42
1:A:635:SER:HB2	1:A:637:GLU:HG3	2.01	0.42
1:E:40:TYR:CD2	1:E:233:PHE:HB2	2.55	0.42
1:F:72:ASN:ND2	1:F:72:ASN:H	2.18	0.42
1:F:209:THR:HG22	1:F:211:THR:H	1.84	0.42
1:F:319:ASP:OD2	1:F:322:LEU:HB2	2.20	0.42
1:F:392:ALA:O	1:F:551:TRP:CH2	2.50	0.42
1:F:479:VAL:HA	1:F:522:HIS:O	2.20	0.42
1:F:486:ILE:CG1	1:F:515:HIS:HB2	2.50	0.42
1:A:120:LEU:C	1:A:122:PRO:HD2	2.45	0.42
1:A:282:ALA:O	1:A:286:ARG:NH1	2.53	0.42
1:D:193:LEU:O	1:D:197:MET:HG3	2.20	0.42
1:D:349:CYS:O	1:D:497:GLN:HG2	2.20	0.42
1:D:550:GLN:OE1	1:D:550:GLN:N	2.48	0.42
1:E:518:GLY:O	1:E:519:ALA:HB3	2.20	0.42
1:F:492:LEU:O	1:F:493:ALA:CB	2.68	0.42
1:B:489:THR:O	1:B:492:LEU:O	2.38	0.42
1:B:534:ASP:HA	1:B:537:GLN:HB2	2.01	0.42
1:B:620:LEU:CB	2:B:901:FAD:O2	2.67	0.42
1:C:572:ASP:CG	1:C:653:ARG:HH11	2.27	0.42
1:D:31:ASN:OD1	1:D:116:HIS:CE1	2.73	0.42
1:D:313:PRO:HD3	1:D:330:PHE:CE2	2.55	0.42
1:D:313:PRO:HD3	1:D:330:PHE:CE1	2.55	0.42
1:E:277:ALA:HB1	1:E:415:VAL:CG1	2.50	0.42
1:E:298:ALA:HB1	1:E:299:PRO:HD2	2.02	0.42
1:E:450:GLN:OE1	1:E:450:GLN:HA	2.20	0.42
1:E:484:SER:HB2	1:E:517:ILE:HG22	2.01	0.42
1:F:144:ASP:HB3	1:F:147:ARG:HB3	2.02	0.42
1:A:55:HIS:NE2	1:A:57:HIS:HB2	2.35	0.41
1:C:340:LEU:HD12	1:C:341:PRO:HD2	2.01	0.41
1:D:144:ASP:O	1:D:147:ARG:HB2	2.20	0.41
1:D:329:ALA:O	1:D:333:ALA:HB2	2.20	0.41
1:D:504:TYR:CE2	1:D:519:ALA:HB2	2.55	0.41
1:D:620:LEU:HD13	2:D:901:FAD:N1	2.35	0.41
1:F:313:PRO:HB3	1:F:330:PHE:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ARG:O	1:A:572:ASP:CG	2.62	0.41
1:B:49:GLU:HG2	1:B:50:VAL:N	2.35	0.41
1:B:354:LEU:HD21	1:B:499:LEU:HD22	2.02	0.41
1:C:584:GLU:HG2	1:F:381:GLU:CG	2.50	0.41
1:D:209:THR:CG2	1:D:211:THR:HG22	2.50	0.41
1:D:264:LYS:HD2	1:D:455:SER:HB3	2.01	0.41
1:D:279:LEU:CD2	1:D:458:VAL:HG11	2.50	0.41
1:E:133:MET:HA	1:E:134:PRO:HD3	1.80	0.41
1:F:498:VAL:HG22	1:F:507:PRO:HD3	2.02	0.41
1:C:441:CYS:HB2	1:C:454:HIS:O	2.20	0.41
1:C:581:PRO:HD3	1:C:651:PRO:HB2	2.02	0.41
1:E:505:LEU:HD13	1:E:517:ILE:HG13	2.02	0.41
1:E:581:PRO:CB	1:E:652:ASN:HB3	2.49	0.41
1:B:120:LEU:O	1:B:121:ALA:C	2.62	0.41
1:B:230:ARG:NH2	1:B:239:MET:CE	2.84	0.41
1:B:391:VAL:HG13	1:B:551:TRP:CE2	2.55	0.41
1:C:43:LEU:CD1	1:C:43:LEU:N	2.82	0.41
1:C:301:LEU:HD13	1:F:109:ASP:HB3	2.03	0.41
1:D:6:ILE:O	1:D:104:PRO:HD2	2.21	0.41
1:D:56:PRO:O	1:D:57:HIS:CD2	2.73	0.41
1:D:489:THR:O	1:D:492:LEU:O	2.38	0.41
1:F:111:ALA:O	1:F:114:HIS:HB3	2.21	0.41
1:F:501:TYR:HE2	1:F:505:LEU:HB2	1.85	0.41
1:A:164:LEU:HD23	1:A:164:LEU:HA	1.93	0.41
1:A:416:LEU:O	1:A:420:GLN:HG3	2.20	0.41
1:A:474:LEU:HD22	1:A:576:MET:CE	2.48	0.41
1:C:570:THR:HG21	1:C:576:MET:HE3	2.02	0.41
1:D:63:ALA:HA	1:D:98:ILE:O	2.21	0.41
1:D:334:ARG:HH12	1:D:402:GLN:CB	2.33	0.41
1:E:530:TYR:CD2	1:E:530:TYR:C	2.98	0.41
1:F:586:THR:O	1:F:590:TYR:HB2	2.20	0.41
1:F:620:LEU:HB2	2:F:901:FAD:O2	2.21	0.41
1:A:132:PRO:HD3	1:A:141:LEU:HD11	2.02	0.41
1:A:316:SER:HB2	1:A:322:LEU:HD23	2.03	0.41
1:C:319:ASP:OD2	1:C:322:LEU:HB2	2.20	0.41
1:D:135:LEU:HD13	1:D:327:SER:HB3	2.03	0.41
1:D:265:ARG:HD3	1:D:265:ARG:HA	1.83	0.41
1:E:250:LEU:HA	1:E:251:PRO:HD3	1.91	0.41
1:E:362:HIS:O	1:E:365:ALA:HB3	2.21	0.41
1:E:576:MET:HG2	1:E:653:ARG:NH1	2.34	0.41
1:E:600:ALA:C	1:E:601:VAL:HG23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ALA:C	1:C:184:LYS:HG3	2.45	0.41
1:D:5:SER:O	1:D:6:ILE:HB	2.20	0.41
1:D:230:ARG:O	1:D:238:GLU:HA	2.20	0.41
1:D:250:LEU:HA	1:D:251:PRO:HD3	1.85	0.41
1:A:240:LEU:HA	1:A:240:LEU:HD12	1.80	0.41
1:B:279:LEU:CD2	1:B:458:VAL:HG11	2.50	0.41
1:B:603:ALA:HA	1:B:604:PRO:HD3	1.87	0.41
1:C:377:ALA:HA	1:C:399:THR:O	2.21	0.41
1:C:481:GLY:HA2	1:C:520:SER:O	2.21	0.41
1:C:483:VAL:HG23	2:C:901:FAD:HM72	2.03	0.41
1:D:259:ARG:HB3	1:D:633:GLN:HG3	2.02	0.41
2:E:901:FAD:HM73	2:E:901:FAD:HM81	1.78	0.41
1:F:590:TYR:CB	1:F:659:LEU:HD23	2.51	0.41
1:A:572:ASP:OD1	1:A:572:ASP:C	2.63	0.41
1:B:39:ARG:NH1	1:B:78:GLN:OE1	2.53	0.41
1:C:301:LEU:CD1	1:F:109:ASP:HB3	2.50	0.41
1:C:535:GLN:HG3	1:C:557:VAL:HB	2.03	0.41
1:D:122:PRO:HG2	1:D:123:TRP:CE3	2.56	0.41
1:D:178:ASP:O	1:D:188:MET:HE1	2.21	0.41
1:D:240:LEU:HD23	1:D:240:LEU:HA	1.91	0.41
1:D:479:VAL:HA	1:D:522:HIS:O	2.21	0.41
1:D:537:GLN:HA	1:D:540:GLN:HB3	2.01	0.41
1:D:659:LEU:HD12	1:D:659:LEU:HA	1.89	0.41
1:E:60:PHE:HB2	1:E:92:LEU:CD1	2.51	0.41
1:E:199:ARG:HD3	1:E:251:PRO:HG2	2.02	0.41
1:E:594:ALA:HB2	1:E:662:GLY:C	2.46	0.41
1:F:111:ALA:C	1:F:114:HIS:HB3	2.45	0.41
1:F:277:ALA:HB1	1:F:415:VAL:CG1	2.51	0.41
1:F:504:TYR:CE2	1:F:519:ALA:HB2	2.55	0.41
1:B:465:ILE:HD12	1:B:613:ALA:CB	2.49	0.41
1:B:508:GLN:HA	1:B:514:HIS:O	2.20	0.41
1:E:146:GLY:HA3	1:E:285:ARG:CD	2.44	0.41
1:F:106:THR:O	1:F:107:ARG:C	2.62	0.41
1:A:77:TRP:CD1	1:A:148:VAL:HG21	2.56	0.40
1:A:63:ALA:HA	1:A:98:ILE:O	2.22	0.40
1:C:489:THR:O	1:C:492:LEU:O	2.39	0.40
1:C:505:LEU:HD12	1:C:506:THR:N	2.36	0.40
1:D:24:PHE:CD2	1:D:180:PHE:CE2	3.10	0.40
1:F:140:ARG:HG2	1:F:332:PHE:HE2	1.86	0.40
1:F:177:LEU:O	1:F:209:THR:HG23	2.21	0.40
1:F:301:LEU:HA	1:F:301:LEU:HD12	1.76	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:435:LEU:HD22	1:F:470:GLN:CD	2.46	0.40
1:B:367:MET:O	1:B:370:MET:CG	2.69	0.40
1:C:304:SER:O	1:C:408:PRO:HB2	2.21	0.40
1:C:437:ARG:HH11	1:C:442:TRP:NE1	2.18	0.40
1:D:11:LEU:CD1	1:D:20:VAL:O	2.69	0.40
1:D:21:SER:OG	1:D:180:PHE:CE1	2.74	0.40
1:D:255:PRO:HB2	1:D:602:SER:HA	2.04	0.40
1:F:87:HIS:N	1:F:87:HIS:HD2	2.15	0.40
1:F:144:ASP:O	1:F:145:GLU:HG2	2.21	0.40
1:F:438:LYS:HG2	1:F:443:LEU:HB2	2.02	0.40
1:A:368:LEU:HD13	1:A:379:ALA:HB2	2.03	0.40
1:B:344:PHE:N	1:B:344:PHE:CD1	2.89	0.40
1:B:489:THR:HB	1:B:490:PRO:CD	2.51	0.40
1:C:131:TRP:CD2	1:C:132:PRO:HD2	2.56	0.40
1:D:34:GLY:HA3	1:D:117:TRP:HZ2	1.87	0.40
1:D:491:GLU:HG2	1:D:551:TRP:CB	2.46	0.40
1:E:517:ILE:HD11	1:E:542:LEU:HD22	2.02	0.40
1:F:435:LEU:HD13	1:F:470:GLN:CD	2.47	0.40
1:A:37:GLU:HG3	1:A:233:PHE:HB3	2.04	0.40
2:A:901:FAD:H9	2:A:901:FAD:H1'2	1.70	0.40
1:F:475:PRO:CB	1:F:654:LEU:HD12	2.51	0.40
1:F:581:PRO:HB3	1:F:652:ASN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	626/688 (91%)	594 (95%)	31 (5%)	1 (0%)	43	76
1	B	626/688 (91%)	600 (96%)	25 (4%)	1 (0%)	43	76
1	C	626/688 (91%)	600 (96%)	25 (4%)	1 (0%)	43	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	655/688 (95%)	599 (92%)	53 (8%)	3 (0%)	24	60
1	E	626/688 (91%)	591 (94%)	33 (5%)	2 (0%)	36	70
1	F	626/688 (91%)	590 (94%)	34 (5%)	2 (0%)	36	70
All	All	3785/4128 (92%)	3574 (94%)	201 (5%)	10 (0%)	36	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	6	ILE
1	E	601	VAL
1	A	519	ALA
1	C	519	ALA
1	D	10	ASN
1	E	237	ARG
1	B	601	VAL
1	D	601	VAL
1	F	605	VAL
1	F	601	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/567 (91%)	490 (95%)	27 (5%)	21	55
1	B	517/567 (91%)	504 (98%)	13 (2%)	42	72
1	C	517/567 (91%)	497 (96%)	20 (4%)	28	62
1	D	546/567 (96%)	513 (94%)	33 (6%)	17	50
1	E	517/567 (91%)	485 (94%)	32 (6%)	16	49
1	F	517/567 (91%)	492 (95%)	25 (5%)	23	57
All	All	3131/3402 (92%)	2981 (95%)	150 (5%)	23	57

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147	ARG
1	A	162	SER
1	A	184	LYS
1	A	239	MET
1	A	240	LEU
1	A	243	VAL
1	A	253	SER
1	A	342	VAL
1	A	358	GLU
1	A	372	LEU
1	A	375	GLU
1	A	391	VAL
1	A	440	ASP
1	A	444	LEU
1	A	453	THR
1	A	473	THR
1	A	531	SER
1	A	537	GLN
1	A	576	MET
1	A	579	ASN
1	A	589	GLU
1	A	595	GLU
1	A	596	GLN
1	A	605	VAL
1	A	644	SER
1	A	656	VAL
1	A	661	LYS
1	B	62	VAL
1	B	168	LEU
1	B	207	LEU
1	B	209	THR
1	B	307	ARG
1	B	358	GLU
1	B	375	GLU
1	B	380	VAL
1	B	391	VAL
1	B	444	LEU
1	B	479	VAL
1	B	595	GLU
1	B	597	LYS
1	C	116	HIS
1	C	141	LEU
1	C	145	GLU

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Mol	Chain	Res	Type
1	C	149	THR
1	C	162	SER
1	C	200	LEU
1	C	207	LEU
1	C	228	GLN
1	C	253	SER
1	C	296	ASP
1	C	354	LEU
1	C	367	MET
1	C	369	SER
1	C	383	ASN
1	C	385	VAL
1	C	508	GLN
1	C	567	ARG
1	C	618	ARG
1	C	635	SER
1	C	644	SER
1	D	2	LYS
1	D	3	HIS
1	D	4	TYR
1	D	10	ASN
1	D	11	LEU
1	D	22	ARG
1	D	32	ASP
1	D	62	VAL
1	D	69	THR
1	D	130	GLN
1	D	141	LEU
1	D	152	LEU
1	D	162	SER
1	D	217	ARG
1	D	334	ARG
1	D	342	VAL
1	D	354	LEU
1	D	368	LEU
1	D	369	SER
1	D	375	GLU
1	D	381	GLU
1	D	387	GLN
1	D	391	VAL
1	D	435	LEU
1	D	453	THR

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Mol	Chain	Res	Type
1	D	474	LEU
1	D	508	GLN
1	D	530	TYR
1	D	532	GLU
1	D	533	ASP
1	D	618	ARG
1	D	653	ARG
1	D	659	LEU
1	E	69	THR
1	E	81	ASP
1	E	141	LEU
1	E	145	GLU
1	E	207	LEU
1	E	229	LYS
1	E	230	ARG
1	E	239	MET
1	E	276	SER
1	E	289	GLN
1	E	320	GLU
1	E	324	ARG
1	E	354	LEU
1	E	372	LEU
1	E	383	ASN
1	E	391	VAL
1	E	393	THR
1	E	413	ARG
1	E	436	SER
1	E	441	CYS
1	E	457	VAL
1	E	458	VAL
1	E	473	THR
1	E	483	VAL
1	E	515	HIS
1	E	517	ILE
1	E	577	VAL
1	E	579	ASN
1	E	587	LEU
1	E	592	SER
1	E	598	ASP
1	E	654	LEU
1	F	87	HIS
1	F	112	LEU

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Mol	Chain	Res	Type
1	F	168	LEU
1	F	177	LEU
1	F	207	LEU
1	F	226	THR
1	F	227	MET
1	F	237	ARG
1	F	243	VAL
1	F	276	SER
1	F	301	LEU
1	F	342	VAL
1	F	345	ASP
1	F	349	CYS
1	F	358	GLU
1	F	370	MET
1	F	388	ILE
1	F	391	VAL
1	F	435	LEU
1	F	440	ASP
1	F	474	LEU
1	F	514	HIS
1	F	521	TYR
1	F	630	LEU
1	F	645	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	GLN
1	A	323	ASN
1	A	361	GLN
1	A	497	GLN
1	A	550	GLN
1	A	579	ASN
1	A	596	GLN
1	A	633	GLN
1	B	47	GLN
1	B	96	HIS
1	B	130	GLN
1	B	221	GLN
1	B	258	ASN
1	B	422	GLN
1	B	464	GLN

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Mol	Chain	Res	Type
1	B	650	ASN
1	C	126	GLN
1	C	221	GLN
1	C	361	GLN
1	C	366	GLN
1	C	383	ASN
1	C	422	GLN
1	C	429	GLN
1	C	550	GLN
1	C	579	ASN
1	C	650	ASN
1	D	3	HIS
1	D	10	ASN
1	D	57	HIS
1	D	114	HIS
1	D	116	HIS
1	D	128	GLN
1	D	308	GLN
1	D	318	HIS
1	D	323	ASN
1	D	383	ASN
1	D	425	GLN
1	D	451	GLN
1	D	515	HIS
1	D	540	GLN
1	E	55	HIS
1	E	91	GLN
1	E	128	GLN
1	E	163	GLN
1	E	538	ASN
1	F	47	GLN
1	F	72	ASN
1	F	87	HIS
1	F	128	GLN
1	F	221	GLN
1	F	383	ASN
1	F	414	ASN
1	F	420	GLN
1	F	431	GLN
1	F	434	ASN
1	F	485	HIS
1	F	536	GLN

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Mol	Chain	Res	Type
1	F	579	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	SO4	D	669	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	B	669	-	4,4,4	0.26	0	6,6,6	0.12	0
3	SO4	C	669	-	4,4,4	0.22	0	6,6,6	0.26	0
3	SO4	A	669	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	670	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	E	669	-	4,4,4	0.24	0	6,6,6	0.11	0
2	FAD	B	901	-	58,58,58	1.10	5 (8%)	85,89,89	1.49	16 (18%)
3	SO4	C	671	-	4,4,4	0.33	0	6,6,6	0.24	0
3	SO4	C	670	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	F	669	-	4,4,4	0.22	0	6,6,6	0.08	0
2	FAD	E	901	-	58,58,58	1.13	5 (8%)	85,89,89	1.54	14 (16%)
2	FAD	C	901	-	58,58,58	1.17	7 (12%)	85,89,89	1.59	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	A	901	-	58,58,58	1.14	5 (8%)	85,89,89	1.59	17 (20%)
3	SO4	A	670	-	4,4,4	0.23	0	6,6,6	0.14	0
2	FAD	D	901	-	58,58,58	1.13	6 (10%)	85,89,89	1.51	16 (18%)
3	SO4	B	670	-	4,4,4	0.24	0	6,6,6	0.06	0
2	FAD	F	901	-	58,58,58	1.15	7 (12%)	85,89,89	1.62	19 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	901	-	-	9/34/50/50	0/6/6/6
2	FAD	E	901	-	-	5/34/50/50	0/6/6/6
2	FAD	C	901	-	-	9/34/50/50	0/6/6/6
2	FAD	A	901	-	-	4/34/50/50	0/6/6/6
2	FAD	D	901	-	-	8/34/50/50	0/6/6/6
2	FAD	F	901	-	-	9/34/50/50	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C4X-N5	3.65	1.38	1.30
2	D	901	FAD	C4X-N5	3.55	1.38	1.30
2	E	901	FAD	C4X-N5	3.51	1.38	1.30
2	F	901	FAD	C4X-N5	3.47	1.38	1.30
2	B	901	FAD	C4X-N5	3.40	1.38	1.30
2	C	901	FAD	C4X-N5	3.34	1.38	1.30
2	F	901	FAD	C10-N1	2.74	1.38	1.33
2	C	901	FAD	P-O3P	2.72	1.62	1.59
2	E	901	FAD	C10-N1	2.71	1.38	1.33
2	E	901	FAD	C2A-N1A	2.69	1.38	1.33
2	E	901	FAD	C2A-N3A	2.65	1.38	1.33
2	C	901	FAD	C2A-N1A	2.63	1.38	1.33
2	A	901	FAD	C10-N1	2.63	1.38	1.33
2	D	901	FAD	C2A-N1A	2.61	1.38	1.33
2	B	901	FAD	C10-N1	2.61	1.38	1.33
2	F	901	FAD	C2A-N3A	2.59	1.38	1.33
2	F	901	FAD	C2A-N1A	2.57	1.38	1.33
2	B	901	FAD	C2A-N1A	2.55	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	901	FAD	C10-N1	2.55	1.38	1.33
2	D	901	FAD	C10-N1	2.51	1.38	1.33
2	D	901	FAD	C2A-N3A	2.49	1.38	1.33
2	C	901	FAD	C2A-N3A	2.46	1.38	1.33
2	A	901	FAD	C2A-N1A	2.41	1.38	1.33
2	A	901	FAD	C2A-N3A	2.35	1.38	1.33
2	C	901	FAD	C8A-N7A	2.28	1.36	1.31
2	F	901	FAD	PA-O3P	2.27	1.62	1.59
2	D	901	FAD	C8A-N7A	2.24	1.36	1.31
2	B	901	FAD	C8A-N7A	2.20	1.35	1.31
2	E	901	FAD	C8A-N7A	2.20	1.35	1.31
2	F	901	FAD	P-O3P	2.19	1.61	1.59
2	C	901	FAD	C5A-N7A	-2.16	1.35	1.39
2	B	901	FAD	C2A-N3A	2.15	1.37	1.33
2	D	901	FAD	P-O3P	2.09	1.61	1.59
2	F	901	FAD	C8A-N7A	2.07	1.35	1.31
2	A	901	FAD	P-O3P	2.06	1.61	1.59

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	FAD	N3A-C2A-N1A	-5.86	119.70	128.58
2	B	901	FAD	N3A-C2A-N1A	-5.84	119.75	128.58
2	C	901	FAD	N3A-C2A-N1A	-5.81	119.78	128.58
2	E	901	FAD	N3A-C2A-N1A	-5.70	119.96	128.58
2	F	901	FAD	N3A-C2A-N1A	-5.48	120.29	128.58
2	D	901	FAD	N3A-C2A-N1A	-5.44	120.34	128.58
2	F	901	FAD	C5A-C4A-N3A	-4.77	120.15	126.72
2	E	901	FAD	C5A-C4A-N3A	-4.66	120.31	126.72
2	C	901	FAD	C5A-C4A-N3A	-4.56	120.44	126.72
2	A	901	FAD	N9A-C8A-N7A	-4.39	107.71	113.94
2	D	901	FAD	C5A-C4A-N3A	-4.04	121.16	126.72
2	D	901	FAD	N9A-C8A-N7A	-4.03	108.21	113.94
2	A	901	FAD	C5A-C4A-N3A	-3.98	121.23	126.72
2	B	901	FAD	N9A-C8A-N7A	-3.91	108.39	113.94
2	C	901	FAD	N9A-C8A-N7A	-3.91	108.39	113.94
2	F	901	FAD	N9A-C8A-N7A	-3.77	108.58	113.94
2	E	901	FAD	N9A-C8A-N7A	-3.76	108.60	113.94
2	A	901	FAD	C5A-N7A-C8A	3.66	109.20	103.45
2	B	901	FAD	C5A-C4A-N3A	-3.51	121.89	126.72
2	D	901	FAD	C5A-N7A-C8A	3.49	108.93	103.45
2	E	901	FAD	C2A-N3A-C4A	3.49	120.34	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	FAD	C2A-N3A-C4A	3.45	120.25	111.83
2	F	901	FAD	C5A-N7A-C8A	3.38	108.77	103.45
2	C	901	FAD	C2A-N3A-C4A	3.38	120.08	111.83
2	C	901	FAD	C5A-N7A-C8A	3.38	108.75	103.45
2	F	901	FAD	C4-N3-C2	-3.37	119.66	125.64
2	A	901	FAD	C2A-N3A-C4A	3.35	120.00	111.83
2	E	901	FAD	C5A-N7A-C8A	3.34	108.70	103.45
2	C	901	FAD	C4-N3-C2	-3.28	119.81	125.64
2	A	901	FAD	C4-N3-C2	-3.23	119.90	125.64
2	F	901	FAD	N3A-C4A-N9A	3.21	132.63	127.17
2	D	901	FAD	C4-N3-C2	-3.18	120.00	125.64
2	B	901	FAD	C5A-N7A-C8A	3.18	108.44	103.45
2	E	901	FAD	N3A-C4A-N9A	3.16	132.54	127.17
2	D	901	FAD	C2A-N3A-C4A	3.13	119.47	111.83
2	F	901	FAD	C5X-C9A-N10	3.12	120.79	117.97
2	C	901	FAD	N3A-C4A-N9A	3.12	132.47	127.17
2	B	901	FAD	C2A-N3A-C4A	3.08	119.35	111.83
2	E	901	FAD	C4-N3-C2	-3.04	120.24	125.64
2	B	901	FAD	C4-N3-C2	-2.98	120.34	125.64
2	A	901	FAD	C9A-C5X-N5	-2.74	119.55	122.45
2	B	901	FAD	C4X-C10-N10	2.73	120.39	116.48
2	F	901	FAD	C4X-C4-N3	2.72	120.17	113.25
2	A	901	FAD	C5X-C9A-N10	2.68	120.39	117.97
2	A	901	FAD	C4X-C4-N3	2.62	119.92	113.25
2	D	901	FAD	C4A-C5A-N7A	-2.61	107.60	110.58
2	E	901	FAD	C5X-C9A-N10	2.59	120.31	117.97
2	B	901	FAD	C10-C4X-N5	-2.59	119.52	124.81
2	C	901	FAD	C5X-C9A-N10	2.59	120.31	117.97
2	D	901	FAD	N3A-C4A-N9A	2.56	131.51	127.17
2	A	901	FAD	N3A-C4A-N9A	2.55	131.50	127.17
2	F	901	FAD	C4X-C10-N1	-2.55	118.35	124.59
2	A	901	FAD	C4A-C5A-N7A	-2.54	107.68	110.58
2	D	901	FAD	C4X-C4-N3	2.54	119.71	113.25
2	E	901	FAD	C4X-C10-N10	2.52	120.09	116.48
2	F	901	FAD	O4-C4-C4X	-2.50	119.94	126.53
2	D	901	FAD	C4X-C10-N10	2.49	120.05	116.48
2	C	901	FAD	C4X-C4-N3	2.46	119.52	113.25
2	D	901	FAD	C5X-C9A-N10	2.43	120.16	117.97
2	E	901	FAD	C4X-C4-N3	2.43	119.44	113.25
2	B	901	FAD	C4X-C4-N3	2.41	119.39	113.25
2	F	901	FAD	C9A-C5X-N5	-2.41	119.90	122.45
2	F	901	FAD	C4A-C5A-N7A	-2.37	107.87	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	FAD	O4-C4-C4X	-2.36	120.30	126.53
2	C	901	FAD	C9A-C5X-N5	-2.34	119.97	122.45
2	C	901	FAD	C6A-C5A-C4A	2.33	120.36	117.18
2	B	901	FAD	C4A-C5A-N7A	-2.33	107.92	110.58
2	C	901	FAD	C5A-C6A-N6A	-2.31	117.57	123.29
2	E	901	FAD	C9A-C5X-N5	-2.31	120.01	122.45
2	C	901	FAD	C4X-C10-N10	2.30	119.78	116.48
2	A	901	FAD	C4A-N9A-C8A	2.29	108.14	105.74
2	A	901	FAD	C10-C4X-N5	-2.29	120.14	124.81
2	C	901	FAD	O4-C4-C4X	-2.28	120.52	126.53
2	D	901	FAD	C9A-C5X-N5	-2.27	120.05	122.45
2	E	901	FAD	C10-C4X-N5	-2.25	120.22	124.81
2	D	901	FAD	C10-C4X-N5	-2.24	120.23	124.81
2	C	901	FAD	C10-C4X-N5	-2.24	120.24	124.81
2	C	901	FAD	C4A-C5A-N7A	-2.22	108.05	110.58
2	E	901	FAD	O4-C4-C4X	-2.21	120.69	126.53
2	A	901	FAD	C4X-C10-N10	2.21	119.65	116.48
2	B	901	FAD	C9A-C5X-N5	-2.21	120.11	122.45
2	F	901	FAD	C4X-C10-N10	2.20	119.64	116.48
2	E	901	FAD	C4A-C5A-N7A	-2.19	108.07	110.58
2	C	901	FAD	C4-C4X-C10	2.18	120.67	116.93
2	C	901	FAD	C4X-C10-N1	-2.15	119.32	124.59
2	B	901	FAD	O2A-PA-O3P	2.14	113.06	107.27
2	C	901	FAD	O2A-PA-O3P	2.14	113.05	107.27
2	F	901	FAD	C4-C4X-C10	2.12	120.56	116.93
2	F	901	FAD	C6A-C5A-C4A	2.11	120.06	117.18
2	A	901	FAD	O2A-PA-O3P	2.10	112.96	107.27
2	A	901	FAD	O4-C4-C4X	-2.10	120.99	126.53
2	D	901	FAD	C4A-N9A-C8A	2.08	107.93	105.74
2	B	901	FAD	N3A-C4A-N9A	2.08	130.71	127.17
2	A	901	FAD	C4X-C10-N1	-2.05	119.58	124.59
2	F	901	FAD	C3B-C2B-C1B	2.04	105.33	101.46
2	F	901	FAD	C1'-N10-C9A	-2.03	116.69	120.63
2	B	901	FAD	O4-C4-C4X	-2.02	121.19	126.53
2	F	901	FAD	C10-C4X-N5	-2.02	120.68	124.81
2	B	901	FAD	C4X-C10-N1	-2.02	119.64	124.59
2	D	901	FAD	O2A-PA-O3P	2.01	112.70	107.27
2	B	901	FAD	C4A-N9A-C8A	2.00	107.84	105.74

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	FAD	PA-O3P-P-O5'
2	B	901	FAD	N10-C1'-C2'-O2'
2	B	901	FAD	N10-C1'-C2'-C3'
2	B	901	FAD	C2'-C3'-C4'-O4'
2	B	901	FAD	C2'-C3'-C4'-C5'
2	B	901	FAD	O3'-C3'-C4'-O4'
2	B	901	FAD	O3'-C3'-C4'-C5'
2	B	901	FAD	O4'-C4'-C5'-O5'
2	C	901	FAD	N10-C1'-C2'-O2'
2	C	901	FAD	O4'-C4'-C5'-O5'
2	D	901	FAD	O4'-C4'-C5'-O5'
2	D	901	FAD	PA-O3P-P-O5'
2	F	901	FAD	C5B-O5B-PA-O2A
2	F	901	FAD	C5B-O5B-PA-O3P
2	F	901	FAD	C2'-C1'-N10-C10
2	F	901	FAD	C1'-C2'-C3'-O3'
2	F	901	FAD	C1'-C2'-C3'-C4'
2	F	901	FAD	O2'-C2'-C3'-O3'
2	F	901	FAD	C3'-C4'-C5'-O5'
2	F	901	FAD	O4'-C4'-C5'-O5'
2	F	901	FAD	O2'-C2'-C3'-C4'
2	C	901	FAD	O2'-C2'-C3'-O3'
2	B	901	FAD	C3'-C4'-C5'-O5'
2	D	901	FAD	C3'-C4'-C5'-O5'
2	A	901	FAD	P-O3P-PA-O1A
2	E	901	FAD	O4'-C4'-C5'-O5'
2	E	901	FAD	PA-O3P-P-O5'
2	C	901	FAD	O2'-C2'-C3'-C4'
2	C	901	FAD	C1'-C2'-C3'-O3'
2	A	901	FAD	N10-C1'-C2'-O2'
2	D	901	FAD	N10-C1'-C2'-O2'
2	E	901	FAD	N10-C1'-C2'-C3'
2	C	901	FAD	P-O3P-PA-O1A
2	D	901	FAD	P-O3P-PA-O1A
2	D	901	FAD	P-O3P-PA-O2A
2	C	901	FAD	O3'-C3'-C4'-C5'
2	B	901	FAD	O4B-C4B-C5B-O5B
2	C	901	FAD	O4B-C4B-C5B-O5B
2	D	901	FAD	O4B-C4B-C5B-O5B
2	E	901	FAD	O4B-C4B-C5B-O5B
2	A	901	FAD	P-O3P-PA-O2A
2	C	901	FAD	O3'-C3'-C4'-O4'
2	E	901	FAD	N10-C1'-C2'-O2'

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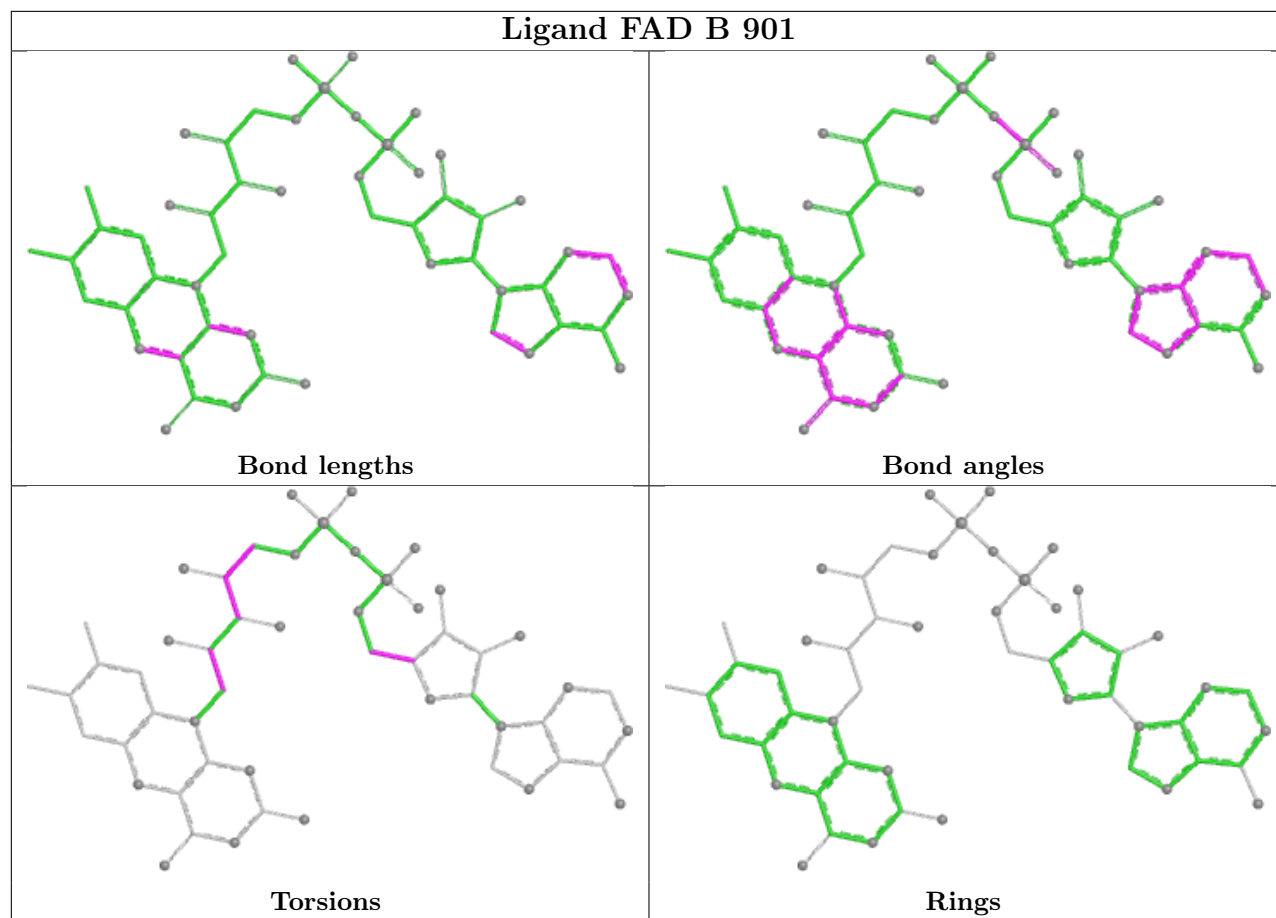
Mol	Chain	Res	Type	Atoms
2	D	901	FAD	O3'-C3'-C4'-C5'

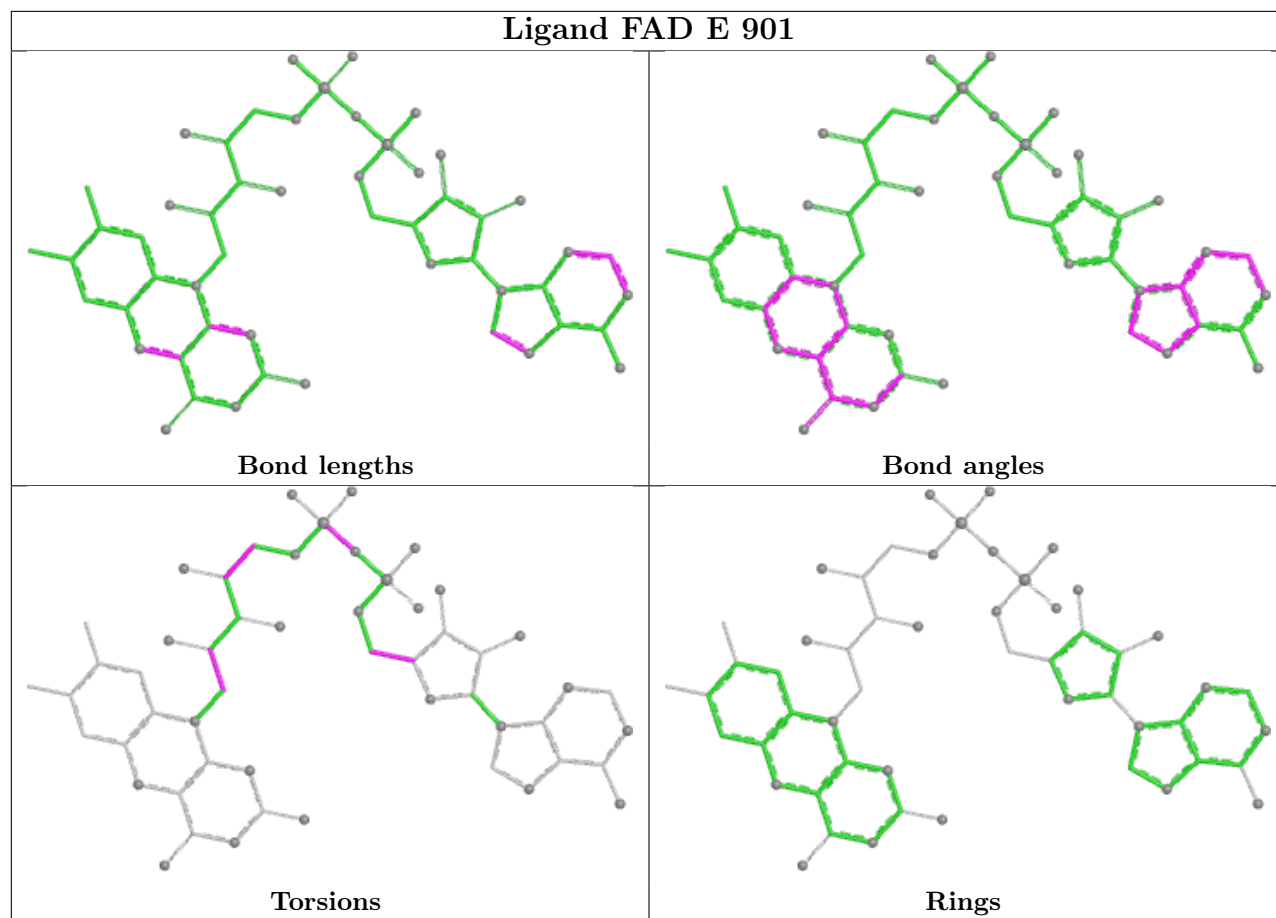
There are no ring outliers.

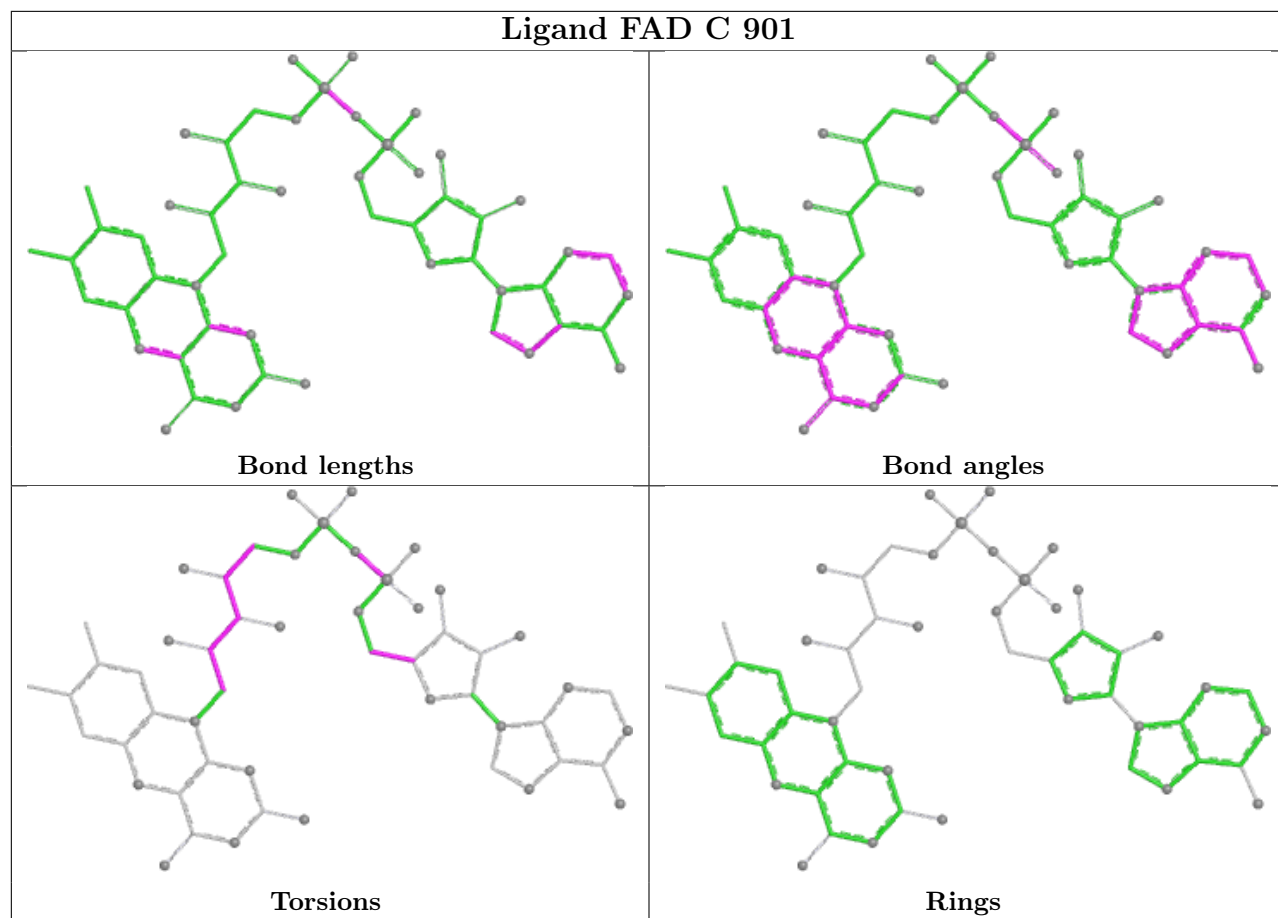
6 monomers are involved in 28 short contacts:

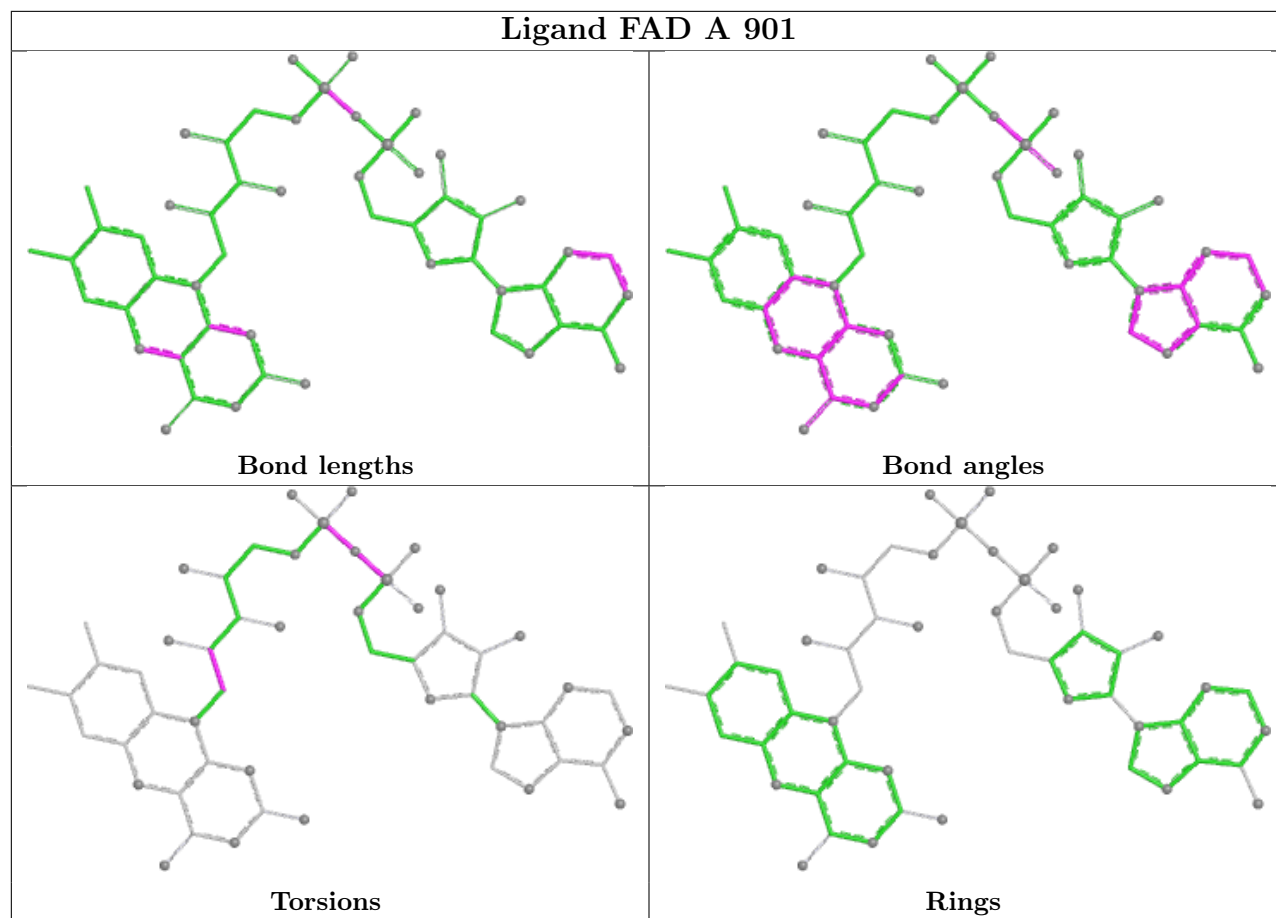
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	901	FAD	5	0
2	E	901	FAD	2	0
2	C	901	FAD	7	0
2	A	901	FAD	6	0
2	D	901	FAD	4	0
2	F	901	FAD	4	0

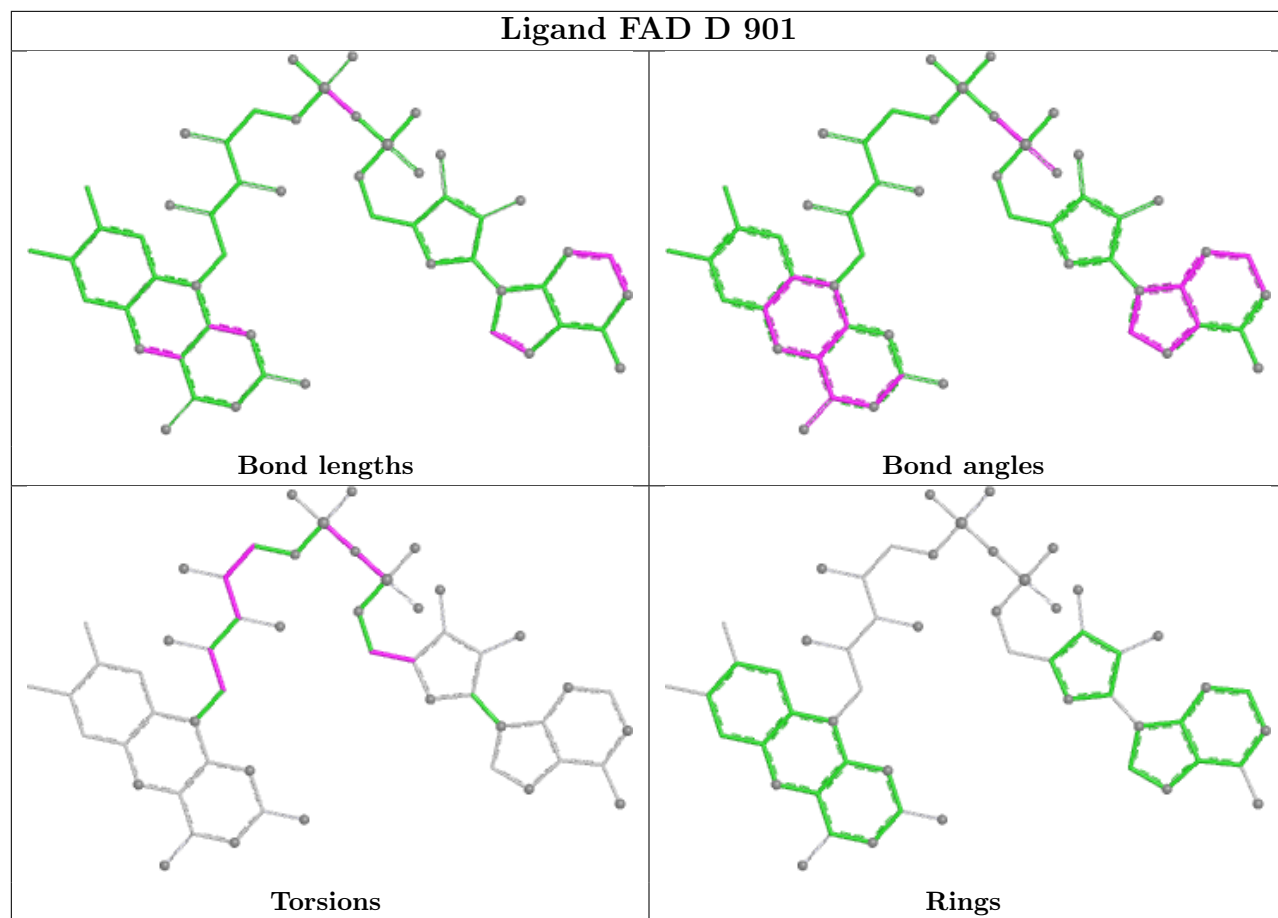
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

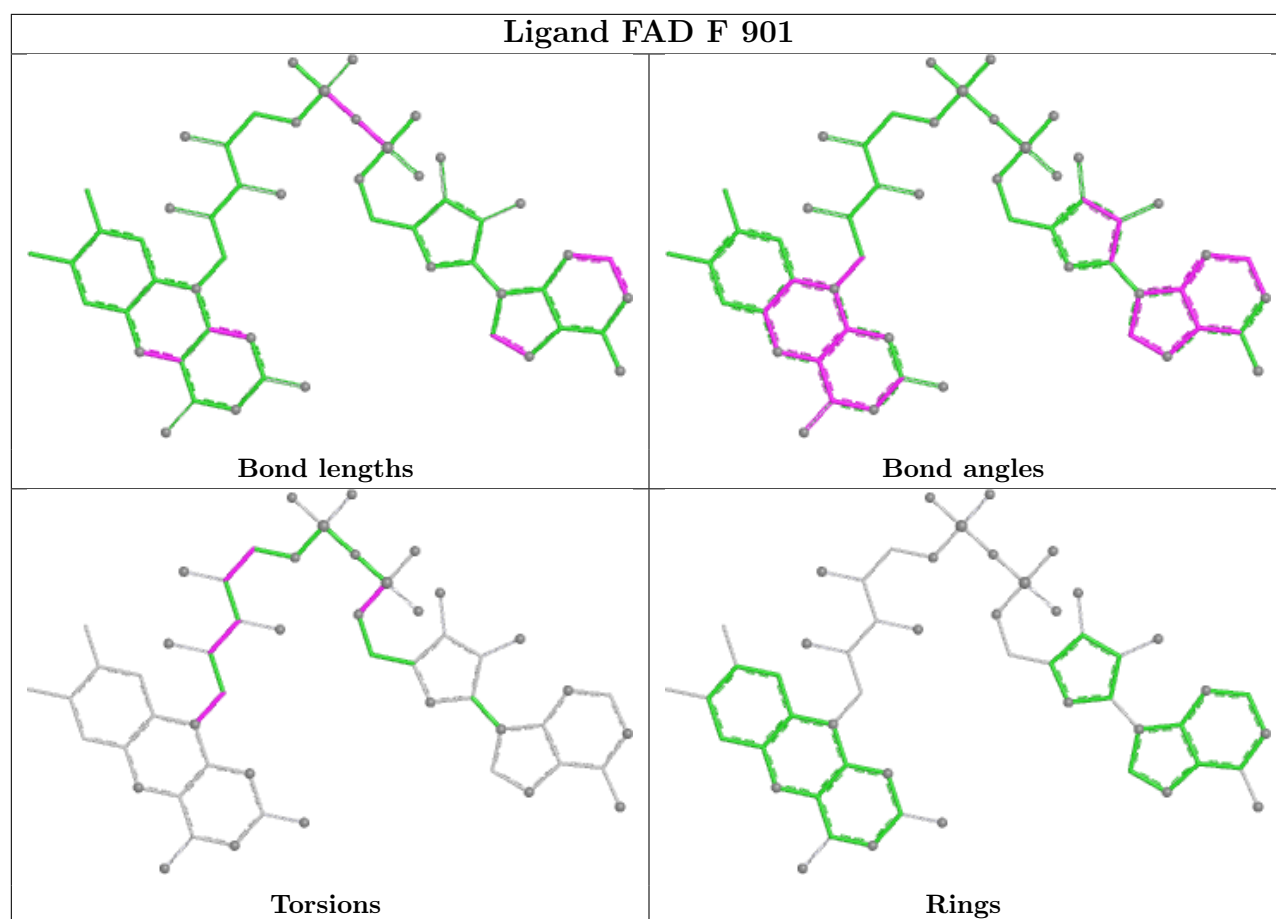












5.7 Other polymers [i](#)

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	628/688 (91%)	-0.43	4 (0%) 85 69	37, 62, 103, 137	0
1	B	628/688 (91%)	-0.50	2 (0%) 90 79	36, 58, 96, 133	0
1	C	628/688 (91%)	-0.43	4 (0%) 85 69	34, 61, 99, 148	0
1	D	659/688 (95%)	0.02	10 (1%) 72 49	44, 84, 143, 180	0
1	E	628/688 (91%)	0.04	5 (0%) 82 64	61, 91, 133, 167	0
1	F	628/688 (91%)	1.19	93 (14%) 5 3	96, 142, 178, 246	0
All	All	3799/4128 (92%)	-0.02	118 (3%) 51 30	34, 78, 155, 246	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	112	LEU	5.5
1	F	168	LEU	4.5
1	F	521	TYR	4.3
1	F	306	ASN	4.2
1	F	483	VAL	4.2
1	D	662	GLY	4.1
1	F	519	ALA	4.0
1	F	654	LEU	3.9
1	F	114	HIS	3.8
1	F	298	ALA	3.8
1	D	4	TYR	3.6
1	F	113	ALA	3.6
1	F	662	GLY	3.5
1	D	599	GLU	3.5
1	C	103	PHE	3.4
1	F	240	LEU	3.4
1	F	379	ALA	3.4
1	F	639	ILE	3.4
1	F	514	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	117	TRP	3.3
1	E	600	ALA	3.3
1	F	314	LEU	3.3
1	F	597	LYS	3.3
1	F	301	LEU	3.2
1	F	248	LEU	3.2
1	F	659	LEU	3.2
1	F	315	LEU	3.1
1	F	387	GLN	3.1
1	A	595	GLU	3.1
1	F	551	TRP	3.0
1	F	151	ASP	3.0
1	F	234	GLY	3.0
1	F	241	CYS	3.0
1	F	285	ARG	2.9
1	D	184	LYS	2.9
1	F	617	SER	2.9
1	F	601	VAL	2.9
1	F	402	GLN	2.9
1	C	318	HIS	2.9
1	A	183	ALA	2.9
1	F	299	PRO	2.9
1	F	363	LYS	2.9
1	F	380	VAL	2.8
1	F	106	THR	2.8
1	F	215	PHE	2.8
1	F	506	THR	2.8
1	F	485	HIS	2.8
1	F	318	HIS	2.7
1	F	250	LEU	2.7
1	F	518	GLY	2.7
1	F	391	VAL	2.7
1	F	486	ILE	2.6
1	F	115	GLN	2.6
1	D	532	GLU	2.6
1	F	102	LYS	2.6
1	F	280	SER	2.6
1	E	252	CYS	2.6
1	F	207	LEU	2.6
1	F	588	VAL	2.6
1	F	428	TYR	2.5
1	A	236	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	526	GLU	2.5
1	F	130	GLN	2.5
1	F	164	LEU	2.5
1	F	309	GLY	2.5
1	F	462	GLY	2.5
1	F	555	VAL	2.5
1	F	110	LEU	2.5
1	D	553	LYS	2.5
1	A	519	ALA	2.4
1	F	124	ALA	2.4
1	F	321	ALA	2.4
1	F	421	GLN	2.4
1	F	58	PRO	2.4
1	F	272	GLY	2.4
1	E	359	LYS	2.4
1	F	557	VAL	2.4
1	F	573	HIS	2.4
1	F	603	ALA	2.4
1	D	597	LYS	2.4
1	C	263	SER	2.4
1	B	658	LYS	2.3
1	F	230	ARG	2.3
1	F	487	PRO	2.3
1	F	269	ILE	2.3
1	F	376	LEU	2.3
1	F	495	LEU	2.3
1	F	435	LEU	2.3
1	F	505	LEU	2.3
1	F	641	MET	2.3
1	F	552	ALA	2.3
1	F	336	PHE	2.3
1	F	307	ARG	2.3
1	F	453	THR	2.2
1	C	359	LYS	2.2
1	F	125	GLU	2.2
1	F	283	LEU	2.2
1	F	660	LEU	2.2
1	F	388	ILE	2.2
1	F	433	GLN	2.2
1	E	657	ARG	2.2
1	E	584	GLU	2.1
1	F	629	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	560	LYS	2.1
1	F	128	GLN	2.1
1	B	600	ALA	2.1
1	D	21	SER	2.1
1	F	504	TYR	2.1
1	F	302	GLY	2.1
1	F	281	LEU	2.1
1	D	183	ALA	2.1
1	F	44	GLY	2.1
1	F	443	LEU	2.1
1	F	127	LEU	2.0
1	F	324	ARG	2.0
1	D	521	TYR	2.0
1	F	64	GLU	2.0
1	F	525	SER	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	F	901	53/53	0.81	0.15	132,162,172,408	0
3	SO4	F	669	5/5	0.81	0.17	162,163,164,165	0
3	SO4	C	671	5/5	0.82	0.18	84,111,116,123	0
3	SO4	D	669	5/5	0.84	0.14	137,140,145,146	0
3	SO4	E	669	5/5	0.88	0.17	123,131,134,137	0
3	SO4	A	670	5/5	0.89	0.16	114,115,120,121	0
3	SO4	C	670	5/5	0.92	0.11	90,104,111,117	0
3	SO4	D	670	5/5	0.94	0.10	96,103,108,116	0

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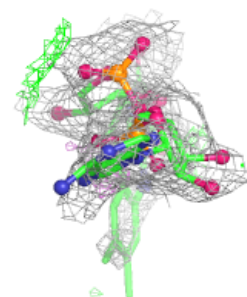
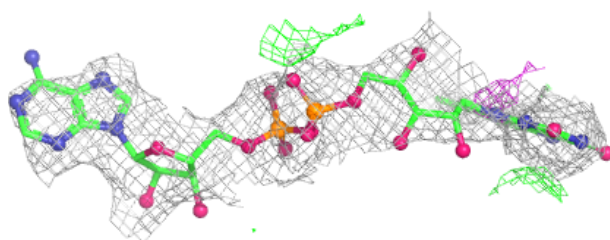
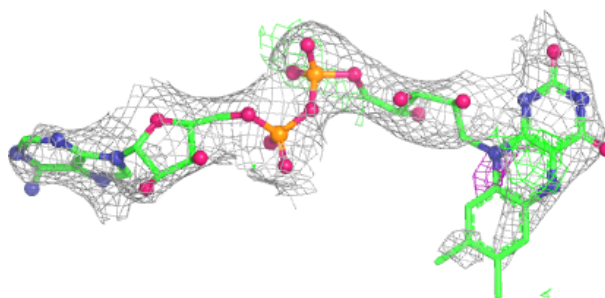
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	D	901	53/53	0.95	0.10	58,85,129,130	0
2	FAD	E	901	53/53	0.95	0.10	48,80,97,137	0
3	SO4	B	670	5/5	0.96	0.11	85,91,94,98	0
2	FAD	C	901	53/53	0.97	0.07	36,54,70,76	0
3	SO4	A	669	5/5	0.97	0.09	75,87,93,95	0
3	SO4	C	669	5/5	0.97	0.09	77,82,87,99	0
3	SO4	B	669	5/5	0.98	0.07	65,74,80,83	0
2	FAD	A	901	53/53	0.98	0.07	32,52,66,71	0
2	FAD	B	901	53/53	0.98	0.07	40,57,75,82	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.

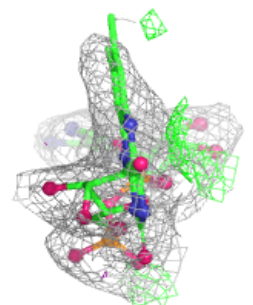
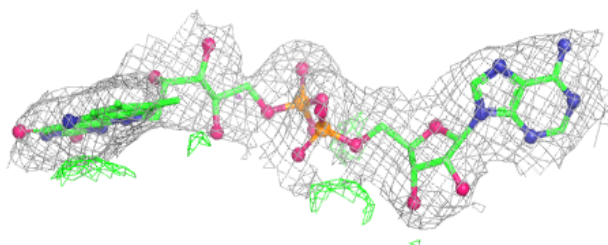
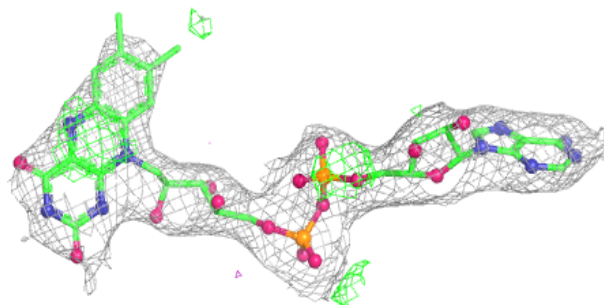
Electron density around FAD F 901:

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

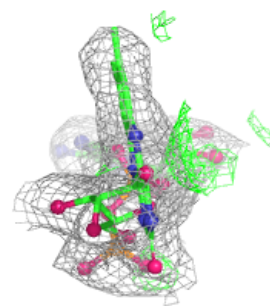
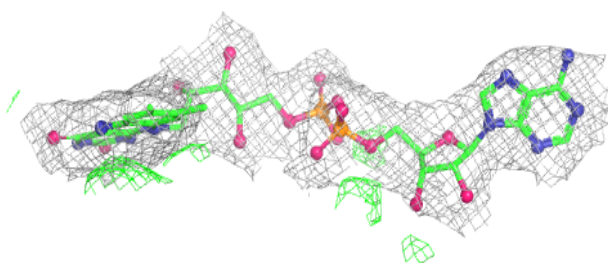
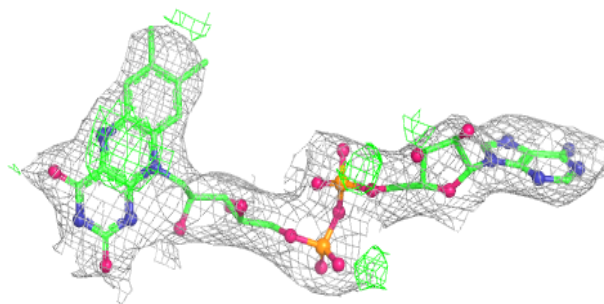


Electron density around FAD D 901:

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

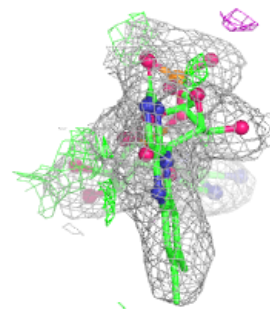
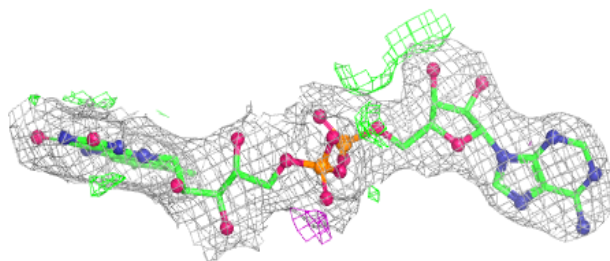
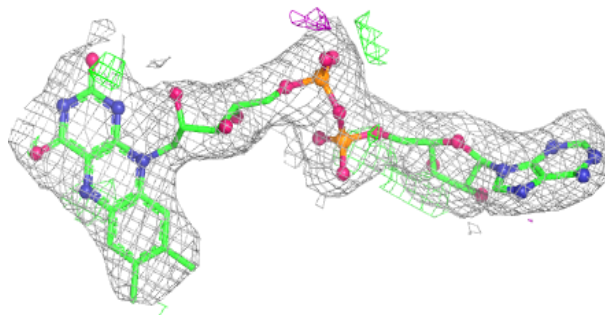
**Electron density around FAD E 901:**

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

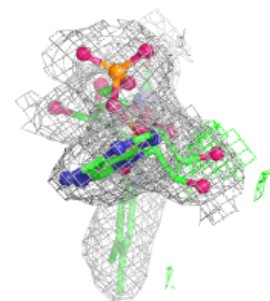
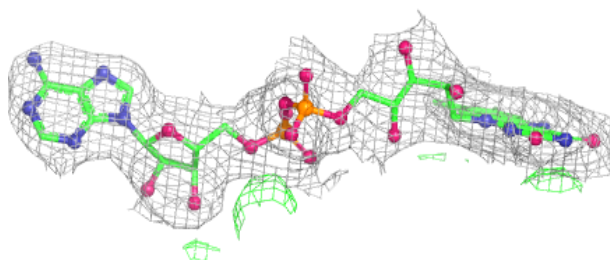
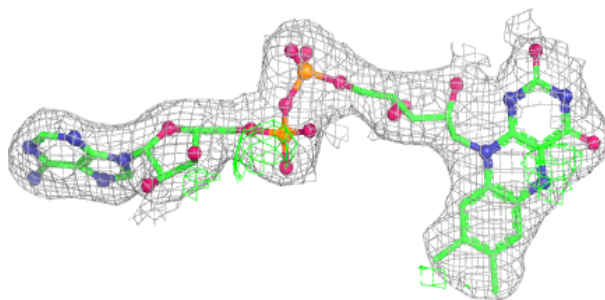


Electron density around FAD C 901:

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

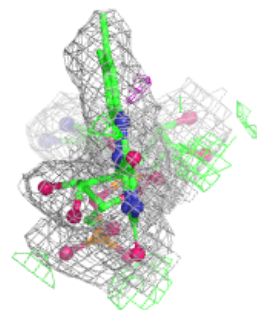
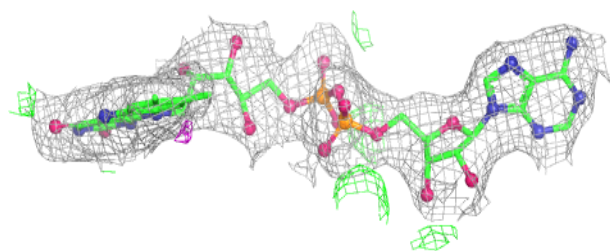
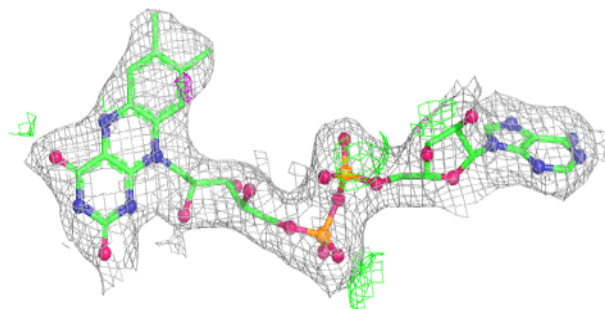
**Electron density around FAD A 901:**

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



Electron density around FAD B 901:

$2mF_o-DF_c$ (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.