



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 10:33 pm BST

PDB ID : 3AWI
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

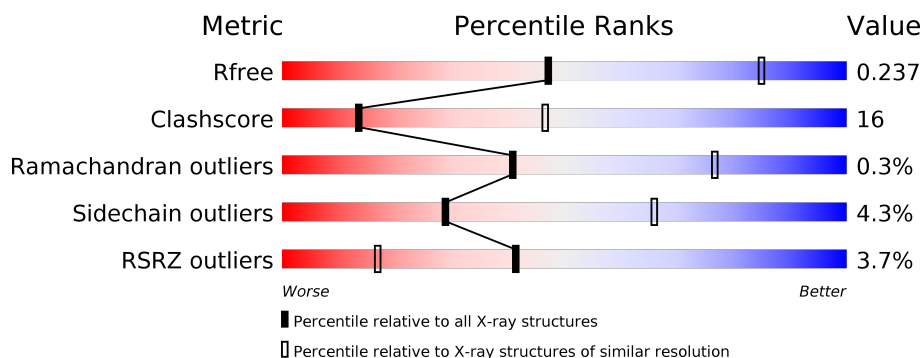
1 Overall quality at a glance

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	<div> <div>68%</div> <div>22%</div> <div>9%</div> </div>
1	B	688	<div> <div>69%</div> <div>22%</div> <div>9%</div> </div>
1	C	688	<div> <div>64%</div> <div>26%</div> <div>9%</div> </div>
1	D	688	<div> <div>59%</div> <div>34%</div> <div>9%</div> </div>
1	E	688	<div> <div>63%</div> <div>26%</div> <div>9%</div> </div>
1	F	688	<div> <div>18%</div> <div>55%</div> <div>34%</div> <div>9%</div> </div>

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 mmmC.

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

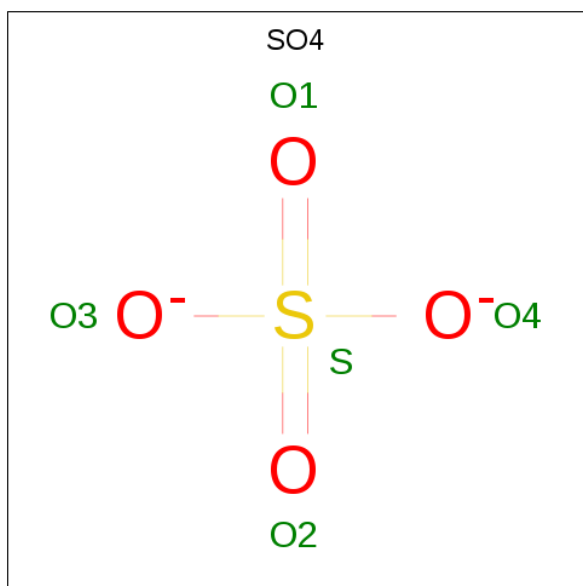
- # FAD

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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 (three-letter code: 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		

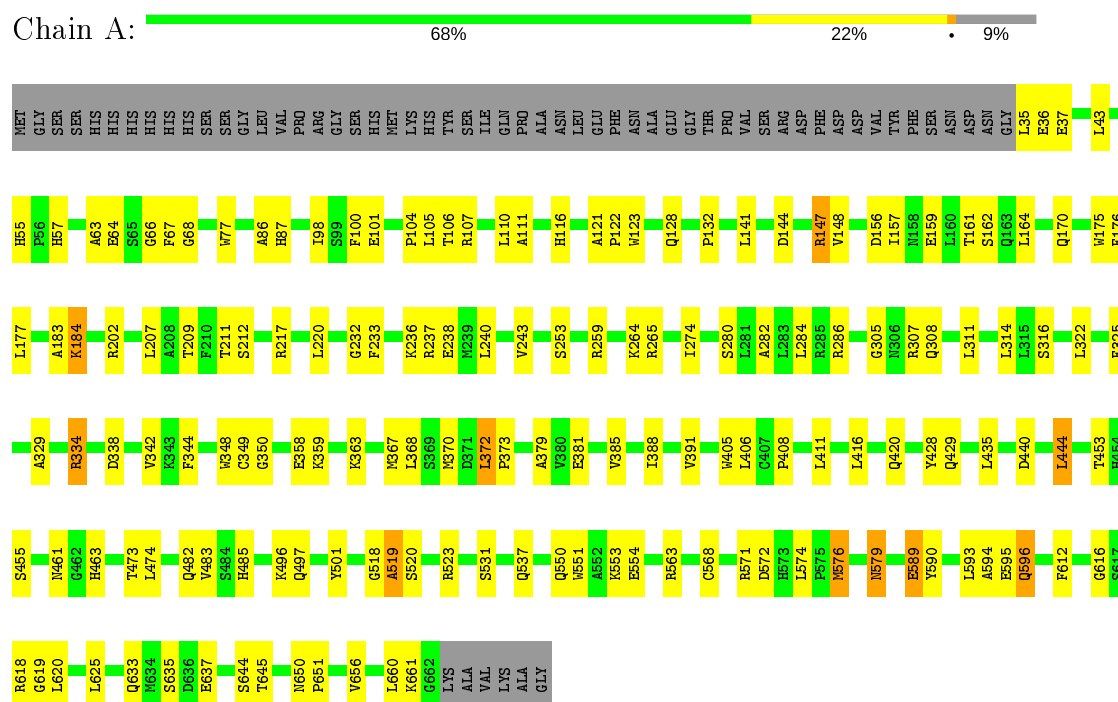
- Molecule 4 is water.

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		

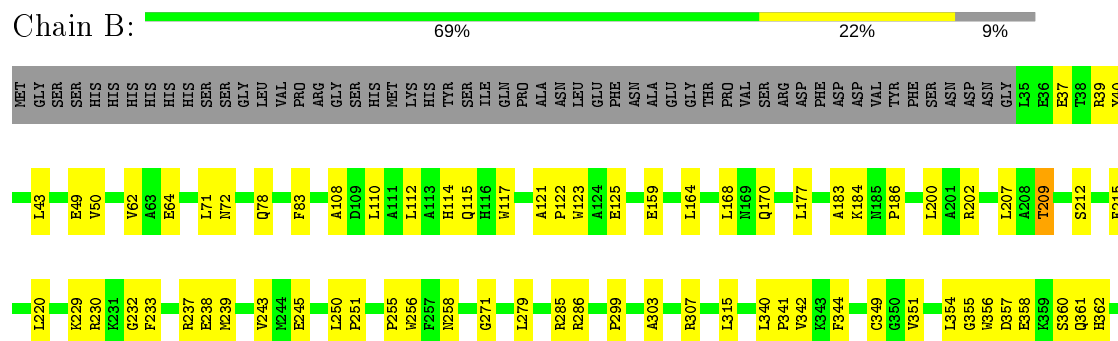
3 Residue-property plots [i](#)

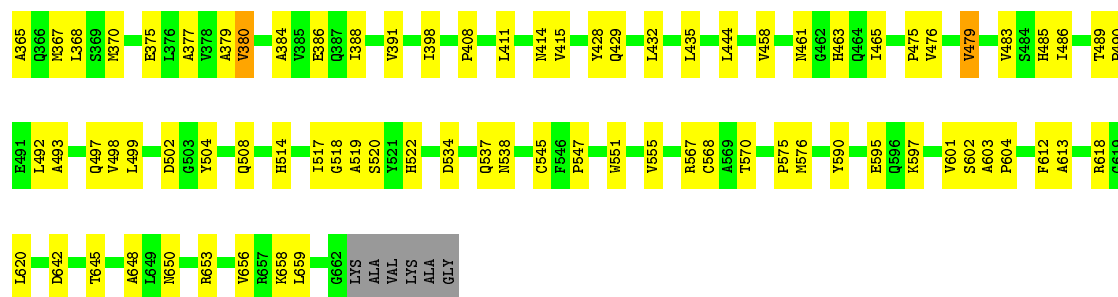
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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



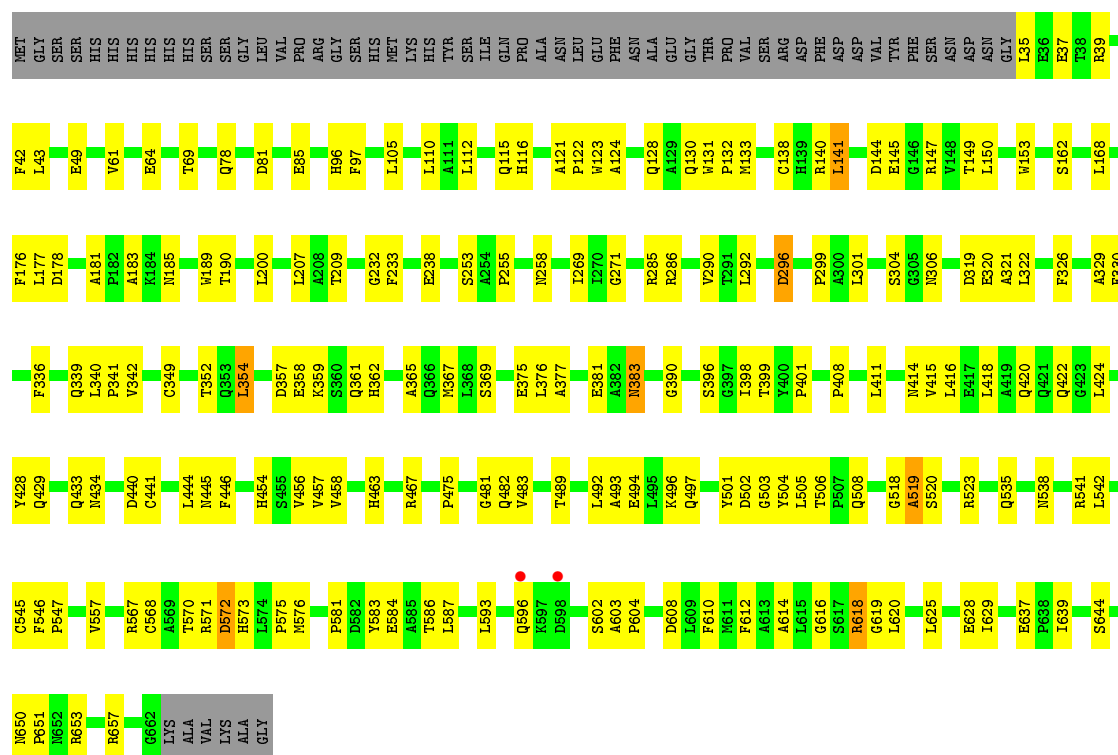
- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC





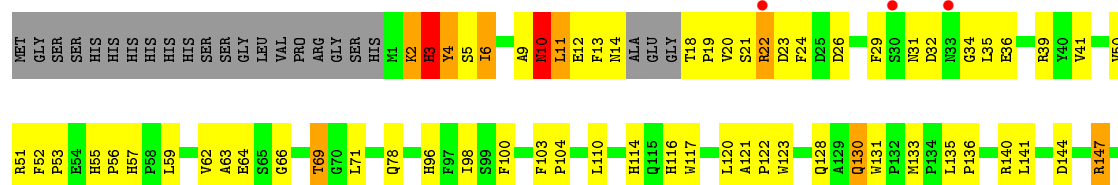
- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC

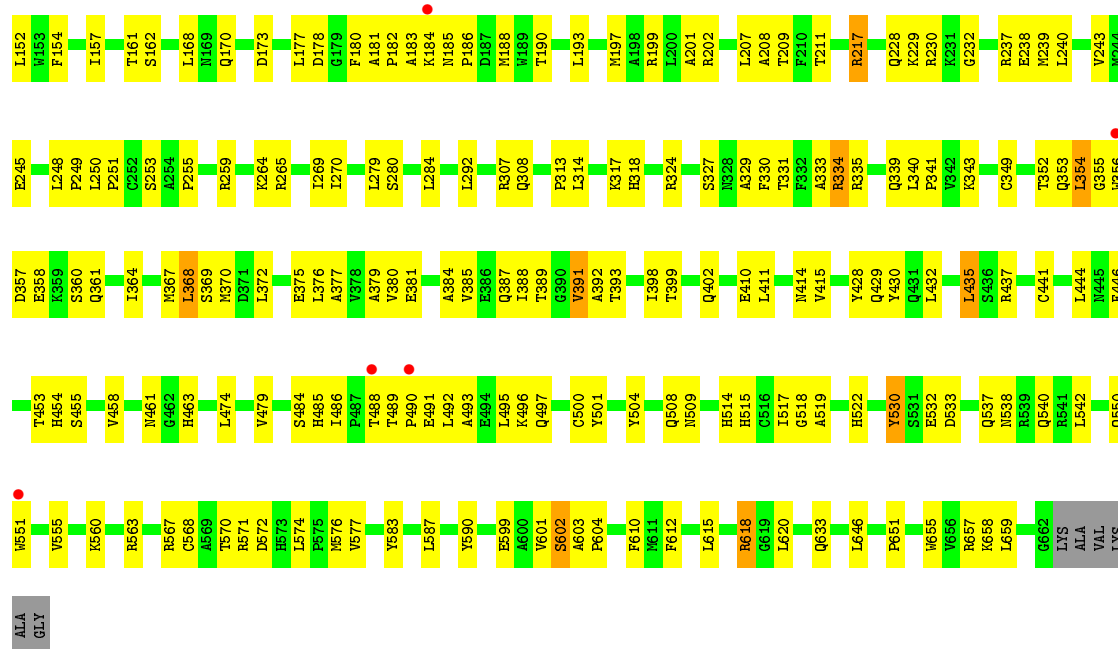
Chain C: 64% 26% 9%



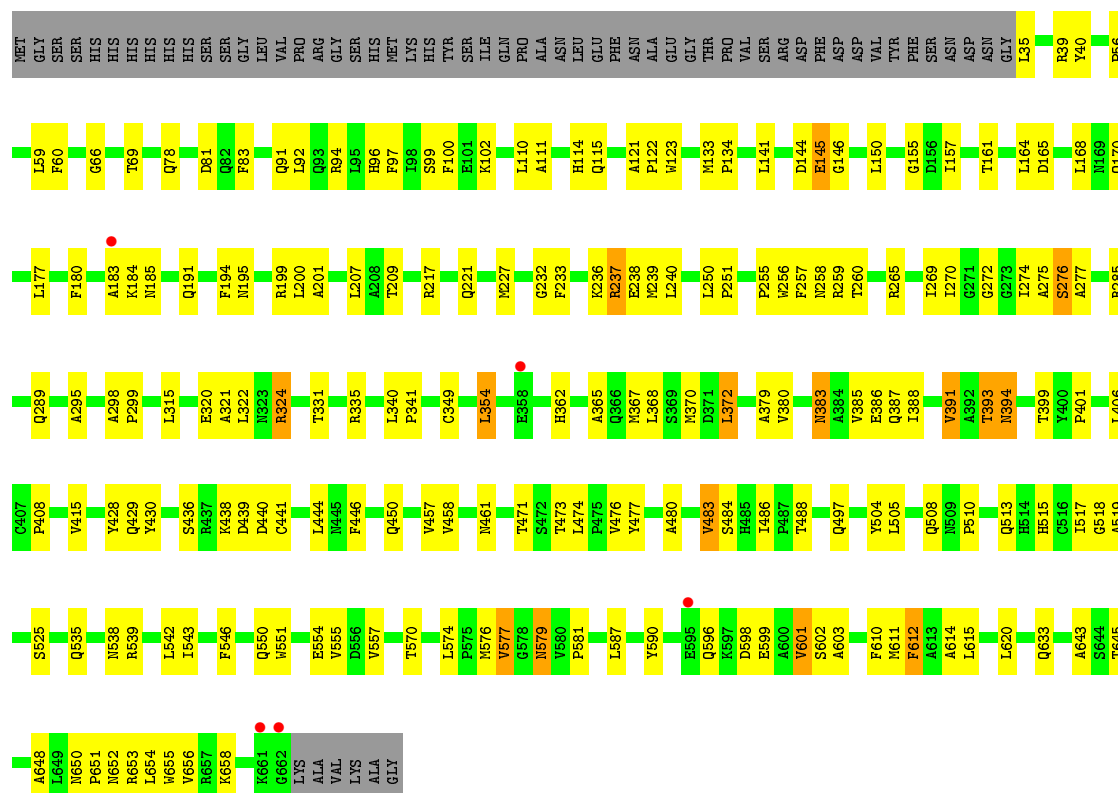
- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC

Chain D: 59% 34% 7%

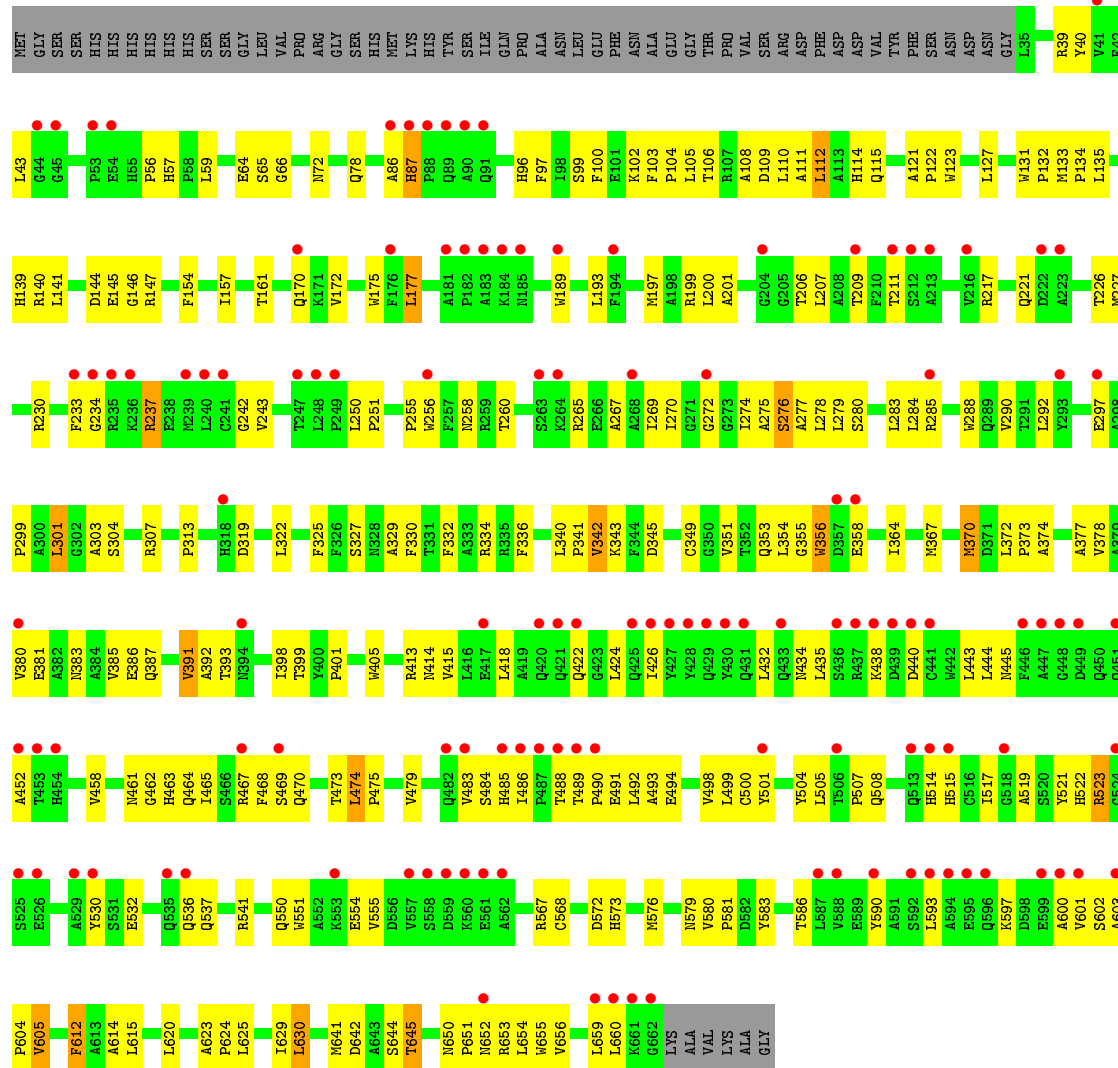




- Molecule 1: tRNA 5-methylaminomethyl-2-thiouridine biosynthesis bifunctional protein mnmC



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



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 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (46.07-3.00) 91.9 (46.07-2.80)	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 0.195 , 0.237	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)	0.31 , 58.5	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 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	0.31	0/5060	0.53	0/6883
1	B	0.32	0/5060	0.53	0/6883
1	C	0.32	0/5060	0.53	0/6883
1	D	0.28	0/5322	0.52	0/7238
1	E	0.27	0/5060	0.47	0/6883
1	F	0.24	0/5060	0.45	0/6883
All	All	0.29	0/30622	0.51	0/41653

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.

There are no bond angle outliers.

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 [i](#)

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4933	0	4777	109	0
1	B	4933	0	4777	116	0
1	C	4933	0	4777	138	0
1	D	5188	0	5004	220	0
1	E	4933	0	4777	151	0
1	F	4933	0	4777	229	0
2	A	53	0	31	7	0
2	B	53	0	31	6	0
2	C	53	0	31	7	0
2	D	53	0	31	4	0
2	E	53	0	31	1	0
2	F	53	0	31	5	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
4	E	1	0	0	0	0
All	All	30287	0	29075	946	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 16.

All (946) 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:HG2	1:E:324:ARG:HH11	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:D:136:PRO:HB2	1:D:324:ARG:HH22	1.35	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HH11	1:D:618:ARG:HG3	1.41	0.85
1:F:270:ILE:HG22	1:F:461:ASN:HB3	1.60	0.83
1:C:618:ARG:CG	1:C:618:ARG:HH11	1.92	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:230:ARG:NH2	1:B:239:MET:HE3	1.96	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
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:D:518:GLY:HA3	1:D:538:ASN:CG	2.03	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:HG3	1:C:618:ARG:HH11	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:232:GLY:HA3	1:D:237:ARG:O	1.91	0.71
1:B:518:GLY:HA3	1:B:538:ASN:CG	2.11	0.71
1:B:230:ARG:HH21	1:B:239:MET:HE3	1.52	0.70
1:F:307:ARG:HB2	1:F:485:HIS:HE1	1.55	0.70
1:E:170:GLN:HA	1:E:201:ALA:O	1.91	0.70
1:E:550:GLN:HG2	1:E:551:TRP:N	2.06	0.70
1:D:133:MET:HE1	1:D:376:LEU:HB2	1.73	0.70
1:D:570:THR:HG21	1:D:574:LEU:O	1.92	0.70
1:F:435:LEU:O	1:F:435:LEU:HD12	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:B:186:PRO:HG3	1:D:253:SER:HB3	1.72	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: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:F:237:ARG:HD2	1:F:237:ARG:H	1.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:35:LEU:HD23	1:D:39:ARG:NH2	2.12	0.65
1:B:232:GLY:N	1:B:238:GLU:HA	2.11	0.65
1:C:207:LEU:C	1:C:207:LEU:HD12	2.17	0.65
1:F:227:MET:CE	1:F:242:GLY:HA3	2.26	0.65
1:A:483:VAL:HG23	2:A:901:FAD:HM72	1.77	0.65
1:A:144:ASP:HB3	1:A:147:ARG:HB2	1.78	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:E:518:GLY:HA3	1:E:538:ASN:CG	2.18	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:140:ARG:C	1:C:141:LEU:HD23	2.18	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:C:483:VAL:HG23	2:C:901:FAD:HM72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:492:LEU:O	1:D:493:ALA:HB3	1.98	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: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:F:464:GLN:HB3	1:F:467:ARG:HD3	1.80	0.63
1:F:97:PHE:CE2	1:F:99:SER:HB2	2.34	0.63
1:D:352:THR:HG22	1:D:399:THR:OG1	1.99	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:NE2	1:A:596:GLN:HA	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:35:LEU:HD11	1:D:120:LEU:HD11	1.81	0.61
1:D:13:PHE:O	1:D:14:ASN:HB3	2.00	0.61
1:C:575:PRO:O	1:C:653:ARG:NH2	2.34	0.61
1:F:135:LEU:HD13	1:F:327:SER:HB3	1.83	0.61
1:F:87:HIS:N	1:F:87:HIS:CD2	2.68	0.61
1:A:308:GLN:HG2	1:A:405:TRP:CE3	2.36	0.61
1:D:571:ARG:O	1:D:572:ASP:CG	2.39	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:D:4:TYR:C	1:D:4:TYR:CD2	2.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:71:LEU:HD13	1:D:117:TRP:CZ3	2.37	0.59
1:B:40:TYR:CE2	1:B:239:MET:HE1	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: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: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:E:207:LEU:HD12	1:E:207:LEU:C	2.24	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:N	1:A:444:LEU:HD23	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:F:297:GLU:CD	1:F:297:GLU:H	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:144:ASP:C	1:E:145:GLU:HG2	2.24	0.57
1:D:51:ARG:O	1:D:55:HIS:HB2	2.04	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:618:ARG:NH1	1:D:618:ARG:CG	2.65	0.57
1:A:106:THR:O	1:A:107:ARG:HB3	2.05	0.57
1:A:461:ASN:HB2	2:A:901:FAD:C8A	2.34	0.57
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: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: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: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: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: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:A:463:HIS:HA	1:A:568:CYS:HB2	1.89	0.55
1:A:64:GLU:HG3	1:A:176:PHE:HB2	1.87	0.55
1:B:428:TYR:O	1:B:429:GLN:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:443:LEU:HA	1:F:452:ALA:O	2.07	0.55
1:C:207:LEU:O	1:C:207:LEU:HD12	2.07	0.55
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:HG3	1:A:184:LYS:O	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:284:LEU:HD23	1:F:422:GLN:CB	2.36	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: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: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:B:435:LEU:CD1	1:B:444:LEU:HD22	2.36	0.54
1:D:334:ARG:CG	1:D:334:ARG:HH11	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:41:VAL:HA	1:D:239:MET:HE1	1.89	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: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
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:272:GLY:H	1:F:276:SER:CB	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:ARG:O	1:F:43:LEU:HB2	2.08	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: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:B:517:ILE:CG1	1:B:518:GLY:H	2.18	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:215:PHE:HB2	1:D:249:PRO:O	2.09	0.53
1:F:370:MET:HE2	1:F:372:LEU:HD11	1.91	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:D:550:GLN:CD	1:D:550:GLN:H	2.11	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:O	1:E:601:VAL:HG12	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:237:ARG:HD2	1:F:237:ARG:N	2.24	0.52
1:F:56:PRO:O	1:F:57:HIS:CG	2.62	0.52
1:A:207:LEU:C	1:A:207:LEU:HD12	2.30	0.52
1:B:362:HIS:O	1:B:365:ALA:HB3	2.10	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:VAL:O	1:C:424:LEU:HD12	2.10	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:489:THR:HB	1:F:490:PRO:HD2	1.92	0.52
1:F:353:GLN:HA	1:F:500:CYS:HB2	1.92	0.52
1:A:122:PRO:HG2	1:A:123:TRP:CE3	2.44	0.51
1:A:259:ARG:HB3	1:A:633:GLN:CD	2.31	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:620:LEU:HG	2:C:901:FAD:C2	2.40	0.51
1:C:286:ARG:HD3	1:C:637:GLU:OE1	2.10	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:A:35:LEU:C	1:A:35:LEU:HD23	2.30	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
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:B:207:LEU:C	1:B:207:LEU:HD12	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:207:LEU:HD12	1:D:207:LEU:C	2.30	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:E:259:ARG:HB3	1:E:633:GLN:CD	2.31	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:A:474:LEU:HD22	1:A:576:MET:HE1	1.93	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:CD2	1:E:515:HIS:N	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:HH11	1:A:286:ARG:HG3	1.76	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:104:PRO:HG3	1:D:154:PHE:CD1	2.47	0.50
1:D:98:ILE:CD1	1:D:168:LEU:HD11	2.42	0.50
1:D:389:THR:O	1:D:495:LEU:HD12	2.11	0.50
1:D:530:TYR:C	1:D:530:TYR:CD2	2.84	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:517:ILE:HD12	1:D:555:VAL:HG11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:HIS:CE1	1:D:563:ARG:HG2	2.47	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:HE21	1:A:596:GLN:HA	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:418:LEU:HD11	1:C:422:GLN:HE21	1.77	0.49
1:C:97:PHE:O	1:C:150:LEU:HD12	2.12	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: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:D:22:ARG:O	1:D:23:ASP:C	2.49	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:C:625:LEU:O	1:C:629:ILE:HG13	2.12	0.49
1:D:184:LYS:O	1:D:185:ASN:HB3	2.11	0.49
1:D:56:PRO:O	1:D:57:HIS:CG	2.66	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:D:50:VAL:O	1:D:53:PRO:HG2	2.12	0.49
1:C:467:ARG:O	1:F:374:ALA:HB1	2.12	0.49
1:F:602:SER:OG	1:F:604:PRO:HD3	2.13	0.49
1:E:315:LEU:HD13	1:E:372:LEU:HD22	1.95	0.49
1:E:483:VAL:HG21	1:E:504:TYR:OH	2.12	0.49
1:E:66:GLY:HA2	1:E:100:PHE:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG	1:F:105:LEU:O	2.12	0.49
1:D:110:LEU:HD22	1:D:131:TRP:CD2	2.48	0.48
1:D:484:SER:HB2	1:D:517:ILE:CG2	2.43	0.48
1:D:259:ARG:NH2	1:D:646:LEU:O	2.45	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:D:10:ASN:N	1:D:10:ASN:HD22	2.11	0.48
1:D:576:MET:HE2	1:D:651:PRO:HA	1.95	0.48
1:E:539:ARG:HG2	1:E:543:ILE:HD13	1.94	0.48
1:B:367:MET:HE1	1:B:398:ILE:HD13	1.96	0.48
1:C:570:THR:HG21	1:C:576:MET:HE2	1.96	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: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:623:ALA:HB3	1:F:624:PRO:HD3	1.95	0.48
1:F:303:ALA:N	2:F:901:FAD:O2A	2.46	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
1:D:370:MET:HG3	1:D:372:LEU:HD21	1.94	0.48
4:C:693:HOH:O	1:F:102:LYS:HE3	2.12	0.48
1:A:36:GLU:H	1:A:36:GLU:CD	2.16	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
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:355:GLY:H	1:F:364:ILE:HD12	1.78	0.48
1:F:299:PRO:HG2	1:F:413:ARG:HG3	1.95	0.48
1:C:138:CYS:HB2	1:C:153:TRP:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:612:PHE:CE2	1:E:615:LEU:HD21	2.45	0.48
1:F:486:ILE:HD12	1:F:555:VAL:HG22	1.95	0.48
1:F:86:ALA:HB3	1:F:87:HIS:HD2	1.78	0.48
1:A:406:LEU:HG	1:A:620:LEU:HD13	1.96	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:O	1:E:557:VAL:HG12	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:A:501:TYR:CD2	1:A:501:TYR:N	2.82	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: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:D:3:HIS:CD2	1:D:3:HIS:O	2.67	0.47
1:E:484:SER:OG	1:E:538:ASN:ND2	2.47	0.47
1:F:250:LEU:H	1:F:250:LEU:HD12	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:428:TYR:O	1:C:429:GLN:HB2	2.14	0.47
1:C:43:LEU:HB3	1:C:49:GLU:OE2	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:F:475:PRO:HG2	1:F:576:MET:CE	2.43	0.47
1:D:181:ALA:O	1:D:183:ALA:O	2.32	0.47
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:F:227:MET:HE3	1:F:242:GLY:HA3	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:LEU:O	1:C:415:VAL:HG23	2.15	0.47
2:C:901:FAD:H1'2	2:C:901:FAD:H9	1.71	0.47
1:C:342:VAL:HG13	1:C:414:ASN:HB3	1.96	0.47
1:F:492:LEU:C	1:F:494:GLU:H	2.17	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:380:VAL:HG22	1:B:384:ALA:HB1	1.97	0.47
1:B:78:GLN:HG3	1:B:123:TRP:CH2	2.49	0.47
1:D:140:ARG:C	1:D:141:LEU:HD23	2.35	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: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:F:475:PRO:HG2	1:F:576:MET:HE3	1.95	0.46
1:F:483:VAL:HG23	2:F:901:FAD:HM72	1.97	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:C:475:PRO:HG2	1:C:576:MET:HE1	1.98	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: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:489:THR:HB	1:F:490:PRO:CD	2.46	0.46
1:F:486:ILE:HG13	1:F:515:HIS:HB2	1.96	0.46
1:F:603:ALA:N	1:F:604:PRO:HD3	2.31	0.46
1:A:175:TRP:HB2	1:A:207:LEU:HB3	1.96	0.46
1:A:66:GLY:HA2	1:A:100:PHE:O	2.16	0.46
1:B:177:LEU:CB	1:B:209:THR:HG23	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:OE2	1:B:72:ASN:HB2	2.15	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: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:F:227:MET:HE2	1:F:242:GLY:HA3	1.97	0.46
1:B:340:LEU:HD12	1:B:341:PRO:HD2	1.97	0.45
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:D:29:PHE:CD2	1:D:117:TRP:CH2	3.04	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:B:315:LEU:HD12	1:B:367:MET:HE2	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
1:B:483:VAL:HG23	2:B:901:FAD:HM72	1.98	0.45
1:C:64:GLU:CB	1:C:176:PHE:HB2	2.46	0.45
1:D:349:CYS:HB2	1:D:496:LYS:O	2.16	0.45
1:D:52:PHE:N	1:D:53:PRO:HD2	2.31	0.45
1:D:587:LEU:HD21	1:D:658:LYS:HZ1	1.81	0.45
1:F:255:PRO:O	1:F:258:ASN:HB2	2.16	0.45
1:F:64:GLU:HG2	1:F:66:GLY:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:518:GLY:CA	1:B:538:ASN:CG	2.84	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:446:PHE:HB2	1:E:450:GLN:HB2	1.99	0.45
1:A:593:LEU:HA	1:A:593:LEU:HD12	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: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:N	1:F:356:TRP:CD1	2.85	0.45
1:F:432:LEU:HD13	1:F:444:LEU:HB3	1.99	0.45
1:A:101:GLU:HA	1:A:101:GLU:OE1	2.17	0.45
1:B:355:GLY:HA2	1:B:360:SER:HB2	1.98	0.45
1:B:258:ASN:HD22	1:B:602:SER:HB2	1.82	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
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:D:655:TRP:O	1:D:659:LEU:HB2	2.16	0.45
1:D:9:ALA:O	1:D:10:ASN:CB	2.65	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:A:593:LEU:O	1:A:594:ALA:C	2.55	0.44
1:B:475:PRO:HG2	1:B:576:MET:CE	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:484:SER:HB2	1:F:517:ILE:CG2	2.47	0.44
1:F:650:ASN:OD1	1:F:651:PRO:HD2	2.17	0.44
1:F:650:ASN:O	1:F:653:ARG:HB2	2.17	0.44
1:F:475:PRO:HB2	1:F:654:LEU:HD12	1.98	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:313:PRO:HD3	1:D:330:PHE:CZ	2.51	0.44
1:D:3:HIS:O	1:D:4:TYR:HB3	2.18	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: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:D:36:GLU:OE1	1:D:36:GLU:HA	2.18	0.44
1:E:260:THR:HB	1:E:579:ASN:ND2	2.32	0.44
1:A:595:GLU:CA	1:E:477:TYR:HB3	2.28	0.44
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:HA	1:D:22:ARG:HD2	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:C:584:GLU:CD	1:F:381:GLU:HB3	2.37	0.44
1:A:579:ASN:H	1:A:579:ASN:HD22	1.65	0.44
1:C:519:ALA:HB3	1:C:538:ASN:CG	2.34	0.44
1:C:545:CYS:C	1:C:547:PRO:HD3	2.38	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:265:ARG:HD3	1:E:265:ARG:HA	1.78	0.44
1:E:256:TRP:HD1	1:E:656:VAL:HG11	1.83	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:NH1	1:A:286:ARG:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:GLN:HA	1:D:201:ALA:O	2.17	0.44
1:D:29:PHE:CG	1:D:117:TRP:CH2	3.06	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:F:233:PHE:CG	1:F:234:GLY:N	2.83	0.44
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:C:381:GLU:OE1	1:C:381:GLU:N	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:B:315:LEU:HD12	1:B:367:MET:CE	2.49	0.43
1:C:189:TRP:CD1	1:C:189:TRP:N	2.86	0.43
1:D:603:ALA:HA	1:D:604:PRO:HD3	1.59	0.43
1:E:354:LEU:CD2	1:E:393:THR:HG21	2.48	0.43
1:F:144:ASP:C	1:F:145:GLU:HG2	2.39	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: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:H	1:C:383:ASN:ND2	2.15	0.43
1:C:572:ASP:CG	1:C:653:ARG:NH1	2.71	0.43
1:F:334:ARG:NH1	1:F:334:ARG:HB3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:642:ASP:CG	1:F:645:THR:HG22	2.39	0.43
1:F:86:ALA:CB	1:F:87:HIS:HD2	2.31	0.43
1:B:411:LEU:O	1:B:415:VAL:HG23	2.19	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:D:307:ARG:HE	1:D:563:ARG:NH2	2.16	0.43
1:E:394:ASN:O	1:E:394:ASN:CG	2.57	0.43
1:F:354:LEU:CD1	1:F:393:THR:HG21	2.48	0.43
2:F:901:FAD:N1	2:F:901:FAD:C2'	2.82	0.43
1:A:329:ALA:HB2	1:A:625:LEU:HD23	2.00	0.43
1:B:230:ARG:HD3	1:B:239:MET:HE2	2.00	0.43
1:D:64:GLU:HG3	1:D:178:ASP:OD1	2.19	0.43
1:D:2:LYS:HA	1:D:2:LYS:HD3	1.82	0.43
1:D:353:GLN:CB	1:D:500:CYS:HB2	2.49	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: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
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:B:43:LEU:N	1:B:43:LEU:CD1	2.82	0.42
1:C:141:LEU:N	1:C:141:LEU:HD23	2.34	0.42
1:F:106:THR:CG2	1:F:108:ALA:HB3	2.50	0.42
1:A:589:GLU:O	1:A:590:TYR:HB2	2.19	0.42
1:A:325:PHE:HB2	1:A:645:THR:CG2	2.49	0.42
1:B:271:GLY:O	2:B:901:FAD:H1B	2.18	0.42
1:C:618:ARG:HG2	1:C:618:ARG:HH11	1.79	0.42
1:D:133:MET:CE	1:D:376:LEU:HB2	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:536:GLN:HB3	1:F:536:GLN:HE21	1.69	0.42
1:A:474:LEU:HD22	1:A:576:MET:CE	2.48	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: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:F:278:LEU:HD22	1:F:336:PHE:CE2	2.55	0.42
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:C:602:SER:O	1:C:603:ALA:C	2.58	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:E:439:ASP:CG	1:E:440:ASP:H	2.23	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:486:ILE:CG1	1:F:515:HIS:HB2	2.50	0.42
1:F:479:VAL:HA	1:F:522:HIS:O	2.20	0.42
1:F:72:ASN:ND2	1:F:72:ASN:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:313:PRO:HD3	1:D:330:PHE:CE2	2.55	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: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:HA	1:E:450:GLN:OE1	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:178:ASP:O	1:D:188:MET:HE1	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
1:B:354:LEU:HD21	1:B:499:LEU:HD22	2.02	0.41
1:B:49:GLU:HG2	1:B:50:VAL:N	2.35	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:279:LEU:CD2	1:D:458:VAL:HG11	2.50	0.41
1:D:41:VAL:HG13	1:D:239:MET:HE2	2.02	0.41
1:D:264:LYS:HD2	1:D:455:SER:HB3	2.01	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:545:CYS:C	1:B:547:PRO:HD3	2.41	0.41
1:B:391:VAL:HG13	1:B:551:TRP:CE2	2.55	0.41
1:C:301:LEU:HD13	1:F:109:ASP:HB3	2.03	0.41
1:C:43:LEU:CD1	1:C:43:LEU:N	2.82	0.41
1:D:6:ILE:O	1:D:104:PRO:HD2	2.21	0.41
1:D:489:THR:O	1:D:492:LEU:O	2.38	0.41
1:D:56:PRO:O	1:D:57:HIS:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:164:LEU:HD23	1.93	0.41
1:A:416:LEU:O	1:A:420:GLN:HG3	2.20	0.41
1:D:334:ARG:HH12	1:D:402:GLN:CB	2.33	0.41
1:D:63:ALA:HA	1:D:98:ILE:O	2.21	0.41
1:F:112:LEU:C	1:F:114:HIS:N	2.73	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:HA	1:D:265:ARG:HD3	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: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:D:357:ASP:CG	1:D:358:GLU:N	2.74	0.41
1:D:5:SER:O	1:D:6:ILE:HB	2.20	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:D:259:ARG:HB3	1:D:633:GLN:HG3	2.02	0.41
1:F:590:TYR:CB	1:F:659:LEU:HD23	2.51	0.41
1:B:39:ARG:NH1	1:B:78:GLN:OE1	2.53	0.41
1:D:240:LEU:HA	1:D:240:LEU:HD23	1.91	0.41
1:D:514:HIS:C	1:D:515:HIS:HD2	2.23	0.41
1:D:479:VAL:HA	1:D:522:HIS:O	2.21	0.41
1:D:659:LEU:HD12	1:D:659:LEU:HA	1.89	0.41
1:E:199:ARG:HD3	1:E:251:PRO:HG2	2.02	0.41
1:C:301:LEU:CD1	1:F:109:ASP:HB3	2.50	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: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:537:GLN:HA	1:D:540:GLN:HB3	2.01	0.41
1:E:60:PHE:HB2	1:E:92:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:77:TRP:CD1	1:A:148:VAL:HG21	2.56	0.40
1:B:230:ARG:HD3	1:B:239:MET:CE	2.51	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:E:518:GLY:CA	1:E:538:ASN:CG	2.87	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
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:D:21:SER:OG	1:D:180:PHE:CE1	2.74	0.40
1:D:11:LEU:CD1	1:D:20:VAL:O	2.69	0.40
1:D:255:PRO:HB2	1:D:602:SER:HA	2.04	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:F:572:ASP:O	1:F:573:HIS:HB2	2.21	0.40
1:F:87:HIS:N	1:F:87:HIS:HD2	2.15	0.40
1:A:104:PRO:C	1:A:105:LEU:HD12	2.41	0.40
1:A:368:LEU:HD13	1:A:379:ALA:HB2	2.03	0.40
1:B:344:PHE:CD1	1:B:344:PHE:N	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:A:37:GLU:HG3	1:A:233:PHE:HB3	2.04	0.40
1:A:67:PHE:O	1:A:68:GLY:C	2.60	0.40
2:A:901:FAD:H1'2	2:A:901:FAD:H9	1.70	0.40
1:F:581:PRO:HB3	1:F:652:ASN:HB3	2.03	0.40
1:F:475:PRO:CB	1:F:654:LEU:HD12	2.51	0.40

There are no symmetry-related clashes.

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	626/688 (91%)	594 (95%)	31 (5%)	1 (0%)	47	82
1	B	626/688 (91%)	600 (96%)	25 (4%)	1 (0%)	47	82
1	C	626/688 (91%)	600 (96%)	25 (4%)	1 (0%)	47	82
1	D	655/688 (95%)	599 (92%)	53 (8%)	3 (0%)	29	68
1	E	626/688 (91%)	591 (94%)	33 (5%)	2 (0%)	41	76
1	F	626/688 (91%)	590 (94%)	34 (5%)	2 (0%)	41	76
All	All	3785/4128 (92%)	3574 (94%)	201 (5%)	10 (0%)	41	76

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%)	495 (96%)	22 (4%)	29	66
1	B	517/567 (91%)	504 (98%)	13 (2%)	47	79
1	C	517/567 (91%)	497 (96%)	20 (4%)	32	69
1	D	546/567 (96%)	515 (94%)	31 (6%)	20	56
1	E	517/567 (91%)	492 (95%)	25 (5%)	25	62
1	F	517/567 (91%)	493 (95%)	24 (5%)	27	64
All	All	3131/3402 (92%)	2996 (96%)	135 (4%)	29	66

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	HIS
1	A	147	ARG
1	A	162	SER
1	A	184	LYS
1	A	243	VAL
1	A	253	SER
1	A	334	ARG
1	A	358	GLU
1	A	372	LEU
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	596	GLN
1	A	612	PHE
1	A	644	SER
1	A	661	LYS
1	B	62	VAL
1	B	83	PHE
1	B	168	LEU
1	B	209	THR
1	B	307	ARG
1	B	358	GLU
1	B	375	GLU
1	B	380	VAL

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Mol	Chain	Res	Type
1	B	479	VAL
1	B	595	GLU
1	B	597	LYS
1	B	612	PHE
1	B	618	ARG
1	C	116	HIS
1	C	141	LEU
1	C	145	GLU
1	C	149	THR
1	C	162	SER
1	C	185	ASN
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	440	ASP
1	C	446	PHE
1	C	508	GLN
1	C	567	ARG
1	C	572	ASP
1	C	612	PHE
1	C	618	ARG
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	147	ARG
1	D	152	LEU
1	D	162	SER
1	D	217	ARG
1	D	334	ARG
1	D	354	LEU
1	D	368	LEU

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Mol	Chain	Res	Type
1	D	369	SER
1	D	375	GLU
1	D	381	GLU
1	D	391	VAL
1	D	435	LEU
1	D	453	THR
1	D	474	LEU
1	D	530	TYR
1	D	532	GLU
1	D	533	ASP
1	D	602	SER
1	D	612	PHE
1	D	618	ARG
1	D	657	ARG
1	E	69	THR
1	E	81	ASP
1	E	145	GLU
1	E	239	MET
1	E	257	PHE
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	394	ASN
1	E	436	SER
1	E	441	CYS
1	E	473	THR
1	E	483	VAL
1	E	577	VAL
1	E	579	ASN
1	E	587	LEU
1	E	598	ASP
1	E	612	PHE
1	E	654	LEU
1	F	87	HIS
1	F	112	LEU
1	F	177	LEU

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Mol	Chain	Res	Type
1	F	207	LEU
1	F	226	THR
1	F	237	ARG
1	F	276	SER
1	F	301	LEU
1	F	342	VAL
1	F	345	ASP
1	F	349	CYS
1	F	356	TRP
1	F	358	GLU
1	F	370	MET
1	F	387	GLN
1	F	391	VAL
1	F	440	ASP
1	F	474	LEU
1	F	514	HIS
1	F	521	TYR
1	F	523	ARG
1	F	612	PHE
1	F	630	LEU
1	F	645	THR

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

Mol	Chain	Res	Type
1	A	130	GLN
1	A	221	GLN
1	A	550	GLN
1	A	579	ASN
1	A	596	GLN
1	B	130	GLN
1	B	221	GLN
1	B	650	ASN
1	C	221	GLN
1	C	318	HIS
1	C	366	GLN
1	C	383	ASN
1	C	422	GLN
1	C	429	GLN
1	C	508	GLN
1	C	550	GLN
1	C	579	ASN

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Mol	Chain	Res	Type
1	C	596	GLN
1	D	7	GLN
1	D	10	ASN
1	D	114	HIS
1	D	116	HIS
1	D	318	HIS
1	D	383	ASN
1	D	414	ASN
1	D	515	HIS
1	E	57	HIS
1	E	91	GLN
1	E	93	GLN
1	E	394	ASN
1	E	538	ASN
1	F	47	GLN
1	F	72	ASN
1	F	87	HIS
1	F	221	GLN
1	F	361	GLN
1	F	383	ASN
1	F	414	ASN
1	F	431	GLN
1	F	445	ASN
1	F	485	HIS
1	F	536	GLN
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 carbohydrates 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	A	669	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	C	670	-	4,4,4	0.15	0	6,6,6	0.09	0
2	FAD	D	901	-	51,58,58	1.35	6 (11%)	60,89,89	1.51	8 (13%)
2	FAD	F	901	-	51,58,58	1.40	6 (11%)	60,89,89	1.71	10 (16%)
3	SO4	B	670	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	D	670	-	4,4,4	0.14	0	6,6,6	0.09	0
3	SO4	B	669	-	4,4,4	0.16	0	6,6,6	0.16	0
3	SO4	E	669	-	4,4,4	0.13	0	6,6,6	0.09	0
3	SO4	C	671	-	4,4,4	0.22	0	6,6,6	0.25	0
3	SO4	C	669	-	4,4,4	0.12	0	6,6,6	0.26	0
3	SO4	F	669	-	4,4,4	0.13	0	6,6,6	0.07	0
3	SO4	D	669	-	4,4,4	0.14	0	6,6,6	0.12	0
2	FAD	E	901	-	51,58,58	1.39	6 (11%)	60,89,89	1.60	9 (15%)
3	SO4	A	670	-	4,4,4	0.13	0	6,6,6	0.12	0
2	FAD	A	901	-	51,58,58	1.37	6 (11%)	60,89,89	1.60	7 (11%)
2	FAD	B	901	-	51,58,58	1.31	6 (11%)	60,89,89	1.59	9 (15%)
2	FAD	C	901	-	51,58,58	1.35	6 (11%)	60,89,89	1.60	7 (11%)

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	D	901	-	-	8/30/50/50	0/6/6/6
2	FAD	F	901	-	-	11/30/50/50	0/6/6/6
2	FAD	B	901	-	-	9/30/50/50	0/6/6/6
2	FAD	E	901	-	-	5/30/50/50	0/6/6/6
2	FAD	A	901	-	-	6/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	901	-	-	9/30/50/50	0/6/6/6

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	FAD	C10-N1	4.29	1.38	1.33
2	E	901	FAD	C10-N1	4.23	1.38	1.33
2	A	901	FAD	C10-N1	4.10	1.38	1.33
2	B	901	FAD	C10-N1	4.08	1.38	1.33
2	E	901	FAD	C2A-N3A	4.06	1.38	1.32
2	F	901	FAD	C2A-N3A	3.99	1.38	1.32
2	C	901	FAD	C10-N1	3.97	1.38	1.33
2	D	901	FAD	C10-N1	3.92	1.38	1.33
2	D	901	FAD	C2A-N3A	3.88	1.38	1.32
2	C	901	FAD	C2A-N3A	3.85	1.38	1.32
2	A	901	FAD	C2A-N3A	3.72	1.38	1.32
2	A	901	FAD	C4X-N5	3.71	1.38	1.33
2	D	901	FAD	C4X-N5	3.56	1.38	1.33
2	B	901	FAD	C2A-N3A	3.51	1.37	1.32
2	E	901	FAD	C4X-N5	3.49	1.38	1.33
2	F	901	FAD	C4X-N5	3.44	1.38	1.33
2	F	901	FAD	C1'-N10	3.42	1.51	1.48
2	B	901	FAD	C4X-N5	3.34	1.38	1.33
2	C	901	FAD	C4X-N5	3.24	1.38	1.33
2	E	901	FAD	C4-N3	2.97	1.38	1.33
2	D	901	FAD	C4-N3	2.94	1.38	1.33
2	F	901	FAD	C4-N3	2.89	1.38	1.33
2	E	901	FAD	C1'-N10	2.85	1.51	1.48
2	C	901	FAD	C4-N3	2.84	1.38	1.33
2	B	901	FAD	C4-N3	2.80	1.37	1.33
2	A	901	FAD	C4-N3	2.71	1.37	1.33
2	D	901	FAD	C1'-N10	2.61	1.50	1.48
2	E	901	FAD	C2A-N1A	2.58	1.38	1.33
2	C	901	FAD	C2A-N1A	2.53	1.38	1.33
2	D	901	FAD	C2A-N1A	2.51	1.38	1.33
2	F	901	FAD	C2A-N1A	2.47	1.38	1.33
2	B	901	FAD	C2A-N1A	2.45	1.38	1.33
2	B	901	FAD	C1'-N10	2.42	1.50	1.48
2	C	901	FAD	C1'-N10	2.34	1.50	1.48
2	A	901	FAD	C2A-N1A	2.32	1.38	1.33
2	A	901	FAD	C1'-N10	2.12	1.50	1.48

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	901	FAD	C1'-N10-C10	6.49	124.22	118.41
2	B	901	FAD	C4-N3-C2	6.16	120.34	115.14
2	E	901	FAD	C4-N3-C2	6.03	120.24	115.14
2	D	901	FAD	C4-N3-C2	5.75	120.00	115.14
2	A	901	FAD	N3A-C2A-N1A	-5.74	119.70	128.68
2	B	901	FAD	N3A-C2A-N1A	-5.71	119.75	128.68
2	C	901	FAD	N3A-C2A-N1A	-5.69	119.78	128.68
2	A	901	FAD	C4-N3-C2	5.63	119.90	115.14
2	E	901	FAD	N3A-C2A-N1A	-5.58	119.96	128.68
2	C	901	FAD	C4-N3-C2	5.53	119.81	115.14
2	F	901	FAD	N3A-C2A-N1A	-5.37	120.29	128.68
2	F	901	FAD	C4-N3-C2	5.35	119.66	115.14
2	D	901	FAD	N3A-C2A-N1A	-5.33	120.34	128.68
2	F	901	FAD	C5X-C9A-N10	4.25	120.79	117.72
2	C	901	FAD	C1'-N10-C10	4.23	122.20	118.41
2	B	901	FAD	C4X-N5-C5X	3.70	120.47	116.77
2	A	901	FAD	C5X-C9A-N10	3.70	120.39	117.72
2	A	901	FAD	C4X-N5-C5X	3.63	120.39	116.77
2	E	901	FAD	C5X-C9A-N10	3.58	120.31	117.72
2	C	901	FAD	C5X-C9A-N10	3.58	120.31	117.72
2	A	901	FAD	C1'-N10-C10	3.50	121.55	118.41
2	D	901	FAD	C5X-C9A-N10	3.38	120.16	117.72
2	C	901	FAD	C4X-N5-C5X	3.35	120.12	116.77
2	F	901	FAD	C4X-N5-C5X	3.15	119.92	116.77
2	E	901	FAD	C4X-N5-C5X	3.15	119.92	116.77
2	D	901	FAD	C4X-N5-C5X	3.14	119.91	116.77
2	E	901	FAD	P-O3P-PA	-3.03	122.42	132.83
2	B	901	FAD	C4X-C4-N3	-2.96	119.39	123.43
2	E	901	FAD	C4X-C4-N3	-2.92	119.44	123.43
2	F	901	FAD	C3B-C2B-C1B	2.89	105.33	100.98
2	C	901	FAD	C4X-C4-N3	-2.86	119.52	123.43
2	B	901	FAD	C5X-C9A-N10	2.72	119.69	117.72
2	D	901	FAD	C4X-C4-N3	-2.72	119.71	123.43
2	B	901	FAD	C1'-N10-C9A	2.65	120.38	118.29
2	A	901	FAD	C4X-C4-N3	-2.57	119.92	123.43
2	E	901	FAD	C3B-C2B-C1B	2.55	104.82	100.98
2	E	901	FAD	C1'-N10-C9A	2.55	120.30	118.29
2	A	901	FAD	P-O3P-PA	-2.52	124.18	132.83
2	B	901	FAD	C10-C4X-N5	-2.51	119.52	121.26
2	D	901	FAD	P-O3P-PA	-2.42	124.52	132.83
2	F	901	FAD	C4X-C4-N3	-2.39	120.17	123.43
2	D	901	FAD	C1'-N10-C9A	2.24	120.06	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	FAD	P-O3P-PA	-2.22	125.20	132.83
2	C	901	FAD	P-O3P-PA	-2.19	125.31	132.83
2	F	901	FAD	P-O3P-PA	-2.18	125.33	132.83
2	F	901	FAD	C9A-N10-C10	-2.17	119.06	121.91
2	D	901	FAD	C1'-N10-C10	2.16	120.34	118.41
2	B	901	FAD	C1B-N9A-C4A	-2.08	122.99	126.64
2	E	901	FAD	C1'-N10-C10	2.04	120.24	118.41
2	F	901	FAD	C1'-N10-C9A	-2.04	116.69	118.29

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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-C9A
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	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	A	901	FAD	PA-O3P-P-O5'
2	C	901	FAD	N10-C1'-C2'-O2'
2	C	901	FAD	O4'-C4'-C5'-O5'
2	F	901	FAD	O2'-C2'-C3'-C4'
2	C	901	FAD	O2'-C2'-C3'-O3'
2	D	901	FAD	C3'-C4'-C5'-O5'
2	B	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	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	D	901	FAD	N10-C1'-C2'-O2'
2	A	901	FAD	N10-C1'-C2'-O2'
2	E	901	FAD	N10-C1'-C2'-C3'
2	C	901	FAD	O2'-C2'-C3'-C4'
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	D	901	FAD	P-O3P-PA-O1A
2	D	901	FAD	P-O3P-PA-O2A
2	C	901	FAD	P-O3P-PA-O1A
2	E	901	FAD	O4B-C4B-C5B-O5B
2	C	901	FAD	O3'-C3'-C4'-C5'
2	F	901	FAD	O4B-C4B-C5B-O5B
2	A	901	FAD	O4'-C4'-C5'-O5'
2	A	901	FAD	O4B-C4B-C5B-O5B
2	A	901	FAD	P-O3P-PA-O2A
2	D	901	FAD	C3B-C4B-C5B-O5B
2	C	901	FAD	C3B-C4B-C5B-O5B
2	E	901	FAD	N10-C1'-C2'-O2'

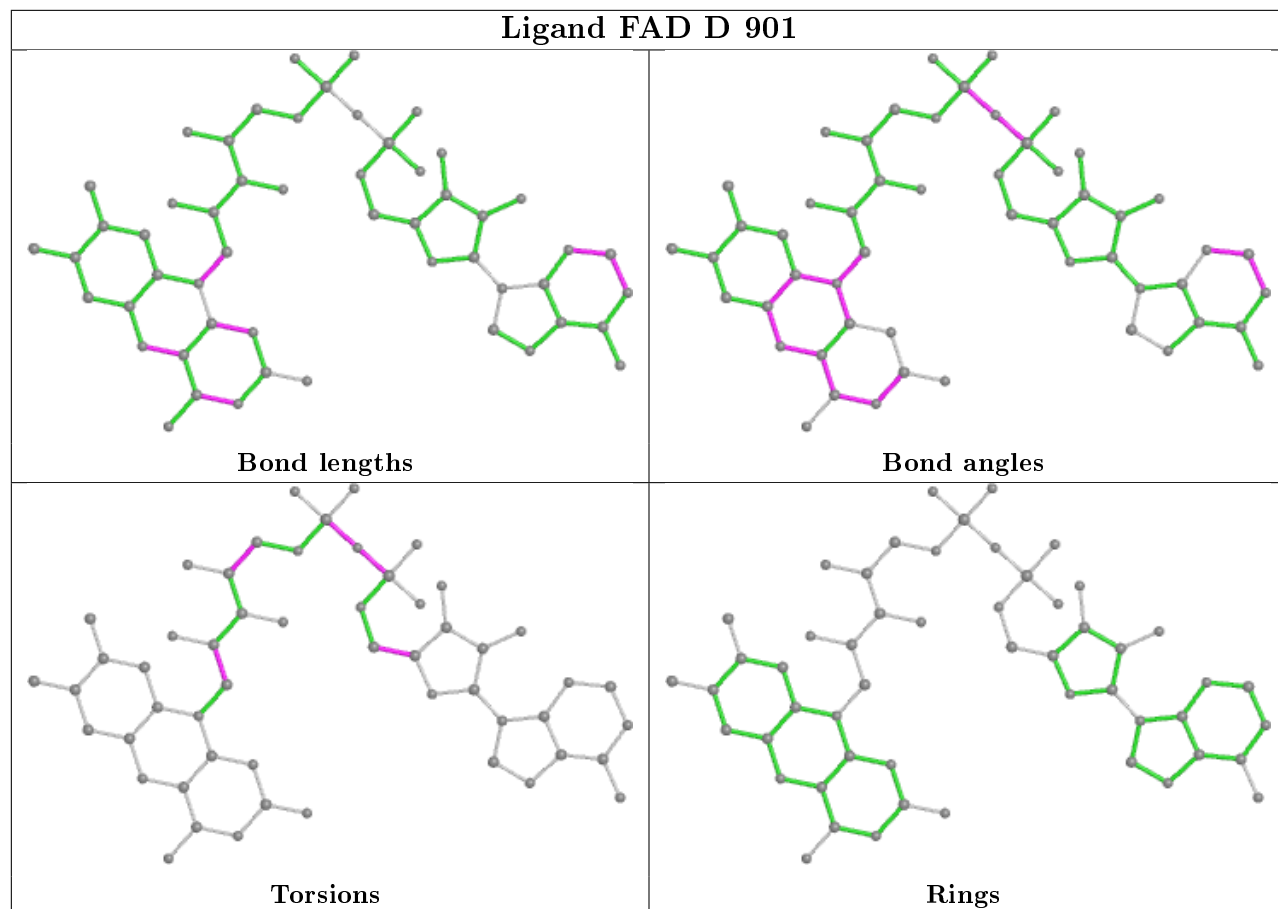
There are no ring outliers.

6 monomers are involved in 30 short contacts:

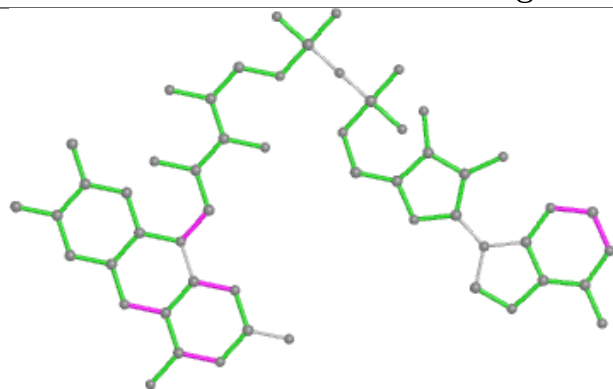
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	901	FAD	4	0
2	F	901	FAD	5	0
2	E	901	FAD	1	0
2	A	901	FAD	7	0
2	B	901	FAD	6	0
2	C	901	FAD	7	0

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

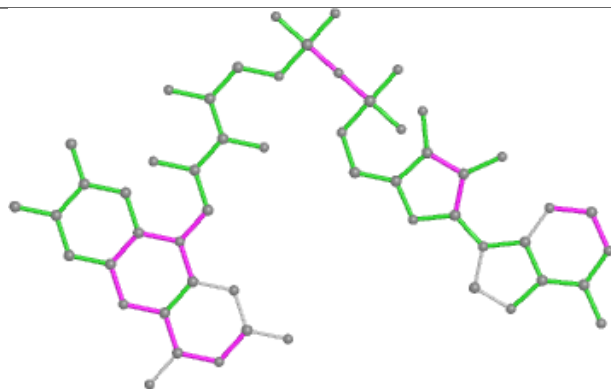
equivalents in the CSD to analyse the geometry.



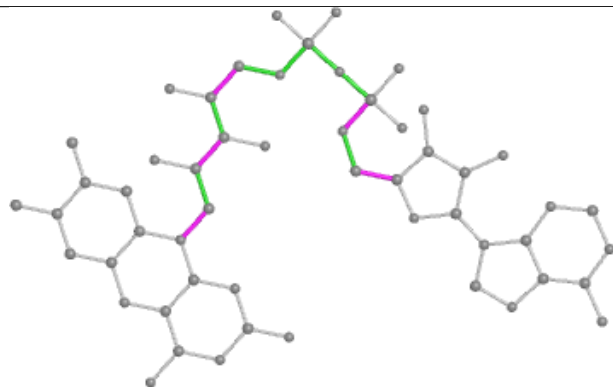
Ligand FAD F 901



Bond lengths



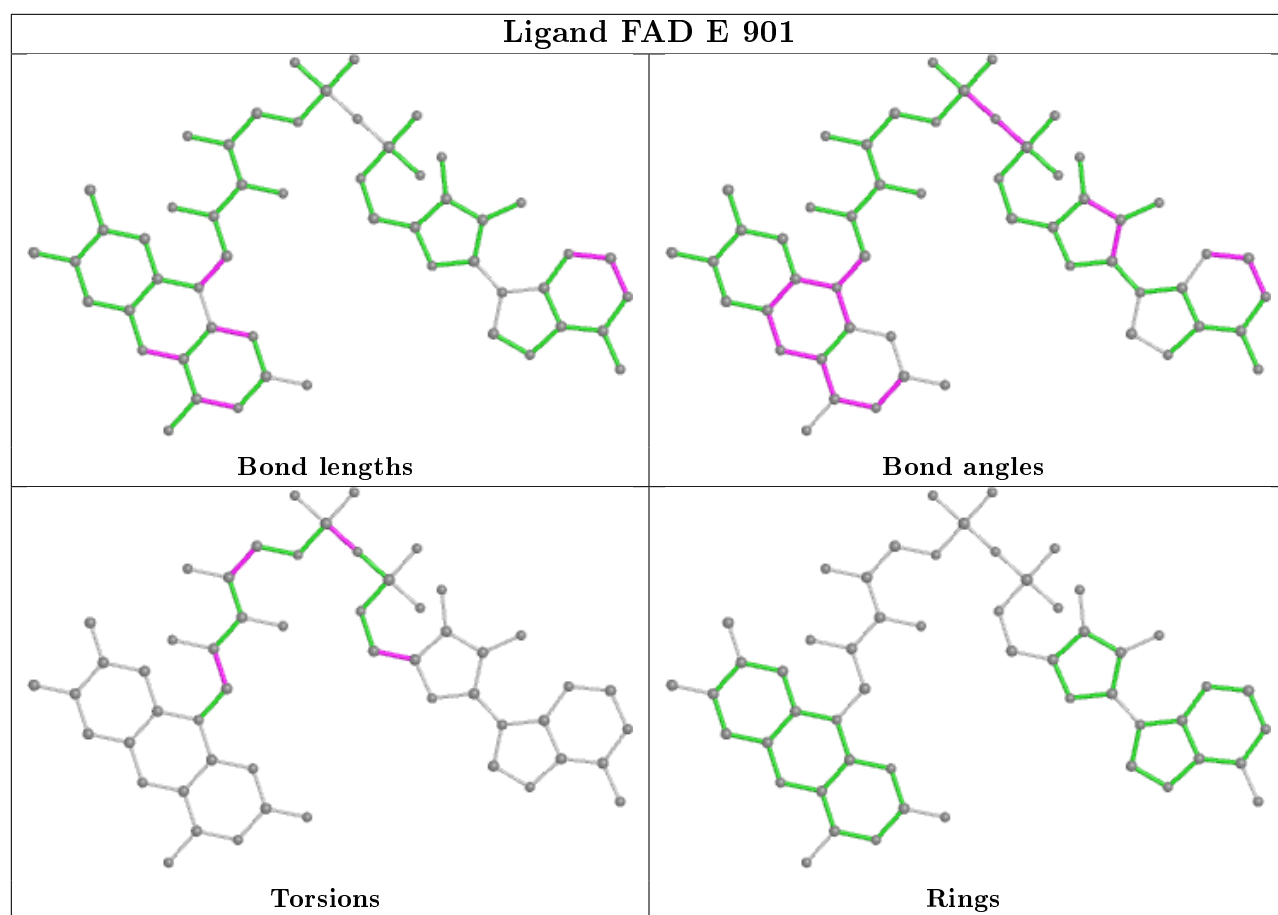
Bond angles

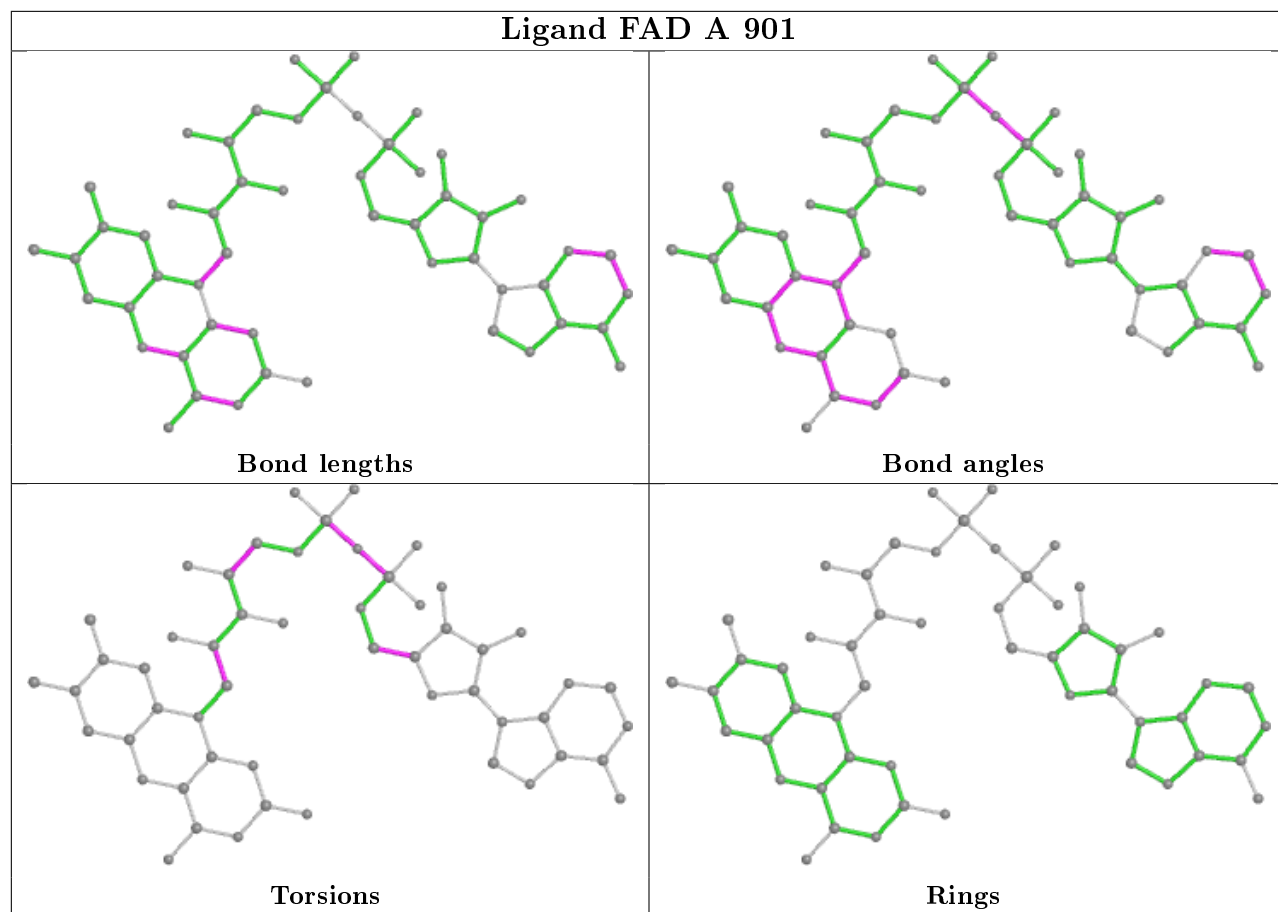


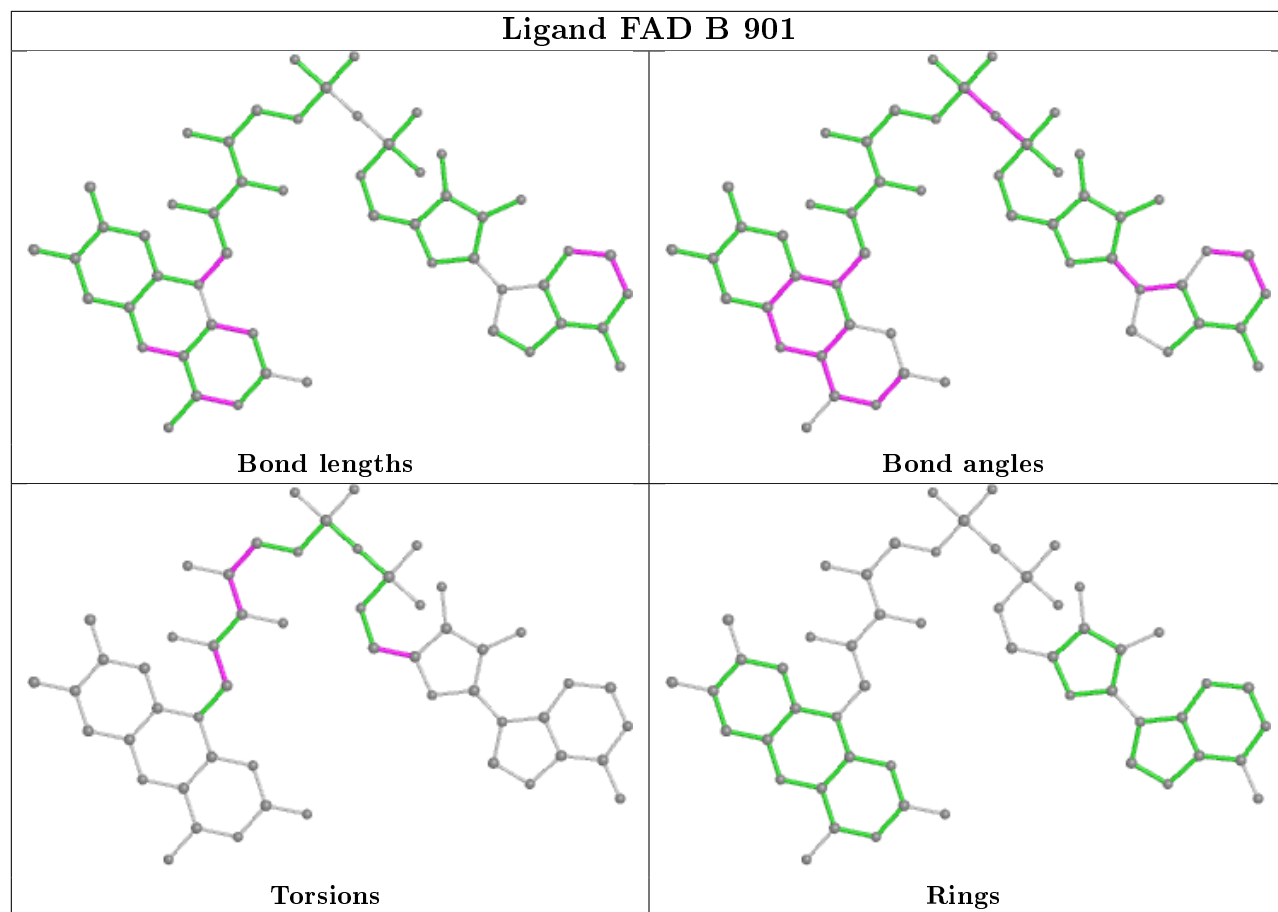
Torsions

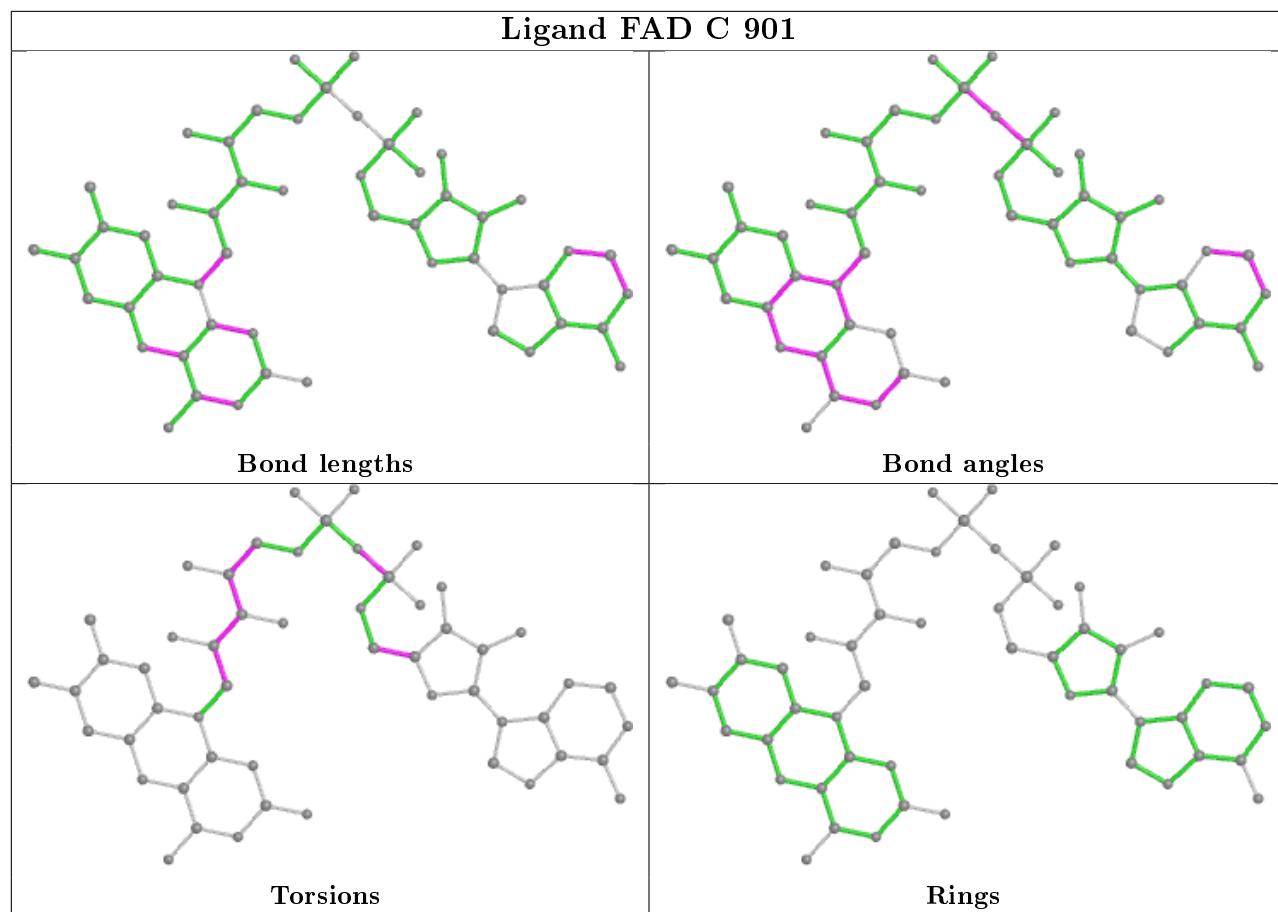


Rings









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%)	-0.58	0	100	100	37, 62, 103, 137	0
1	B	628/688 (91%)	-0.59	0	100	100	36, 58, 96, 133	0
1	C	628/688 (91%)	-0.60	2 (0%)	94	84	33, 61, 99, 148	0
1	D	659/688 (95%)	-0.29	8 (1%)	79	54	44, 84, 143, 180	0
1	E	628/688 (91%)	-0.38	5 (0%)	86	65	61, 91, 133, 167	0
1	F	628/688 (91%)	0.89	124 (19%)	1	0	96, 142, 178, 246	0
All	All	3799/4128 (92%)	-0.26	139 (3%)	41	17	33, 78, 155, 246	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	514	HIS	6.1
1	F	596	GLN	5.5
1	F	588	VAL	5.2
1	F	439	ASP	5.1
1	F	483	VAL	4.7
1	F	235	ARG	4.7
1	F	452	ALA	4.7
1	F	482	GLN	4.7
1	F	487	PRO	4.7
1	F	182	PRO	4.4
1	F	427	TYR	4.3
1	F	433	GLN	4.2
1	F	438	LYS	4.2
1	F	428	TYR	4.1
1	F	515	HIS	4.1
1	F	558	SER	4.1
1	F	263	SER	4.0
1	F	451	GLN	4.0
1	F	239	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	357	ASP	3.9
1	F	592	SER	3.8
1	F	241	CYS	3.8
1	F	234	GLY	3.8
1	F	600	ALA	3.8
1	F	441	CYS	3.8
1	F	91	GLN	3.7
1	F	535	GLN	3.7
1	F	448	GLY	3.6
1	F	562	ALA	3.6
1	F	593	LEU	3.6
1	F	89	GLN	3.6
1	F	447	ALA	3.5
1	F	216	VAL	3.5
1	E	662	GLY	3.5
1	F	183	ALA	3.5
1	F	240	LEU	3.4
1	F	590	TYR	3.3
1	F	601	VAL	3.3
1	F	560	LYS	3.2
1	F	595	GLU	3.2
1	F	248	LEU	3.2
1	F	421	GLN	3.2
1	F	662	GLY	3.2
1	F	430	TYR	3.2
1	F	557	VAL	3.2
1	F	486	ILE	3.2
1	F	425	GLN	3.1
1	F	525	SER	3.1
1	F	449	ASP	3.1
1	E	661	LYS	3.1
1	F	506	THR	3.1
1	F	603	ALA	3.1
1	F	526	GLU	3.0
1	F	660	LEU	3.0
1	F	599	GLU	3.0
1	F	518	GLY	3.0
1	F	90	ALA	3.0
1	F	559	ASP	3.0
1	F	453	THR	3.0
1	F	429	GLN	2.9
1	F	501	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	F	422	GLN	2.9
1	F	204	GLY	2.9
1	F	454	HIS	2.9
1	F	209	THR	2.9
1	F	185	ASN	2.8
1	F	513	GLN	2.8
1	F	170	GLN	2.8
1	D	33	ASN	2.8
1	F	223	ALA	2.8
1	F	293	TYR	2.7
1	F	437	ARG	2.7
1	F	181	ALA	2.7
1	F	594	ALA	2.7
1	F	45	GLY	2.7
1	F	440	ASP	2.7
1	F	358	GLU	2.7
1	F	86	ALA	2.7
1	F	661	LYS	2.6
1	F	536	GLN	2.6
1	F	272	GLY	2.6
1	F	436	SER	2.6
1	F	256	TRP	2.6
1	F	469	SER	2.6
1	F	54	GLU	2.6
1	F	485	HIS	2.6
1	F	431	GLN	2.5
1	D	551	TRP	2.5
1	F	264	LYS	2.5
1	F	213	ALA	2.5
1	F	318	HIS	2.5
1	F	53	PRO	2.5
1	F	426	ILE	2.5
1	F	211	THR	2.4
1	D	490	PRO	2.4
1	E	358	GLU	2.4
1	F	561	GLU	2.4
1	F	553	LYS	2.4
1	F	233	PHE	2.4
1	F	44	GLY	2.4
1	D	184	LYS	2.4
1	F	417	GLU	2.4
1	D	30	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	529	ALA	2.4
1	C	596	GLN	2.4
1	F	247	THR	2.4
1	F	236	LYS	2.4
1	F	297	GLU	2.3
1	F	249	PRO	2.3
1	F	285	ARG	2.3
1	F	490	PRO	2.3
1	F	530	TYR	2.3
1	F	222	ASP	2.3
1	F	184	LYS	2.3
1	F	380	VAL	2.3
1	C	598	ASP	2.2
1	E	183	ALA	2.2
1	D	488	THR	2.2
1	F	488	THR	2.2
1	F	394	ASN	2.2
1	F	268	ALA	2.1
1	F	659	LEU	2.1
1	F	194	PHE	2.1
1	F	524	GLY	2.1
1	F	212	SER	2.1
1	D	22	ARG	2.1
1	D	356	TRP	2.1
1	F	587	LEU	2.1
1	F	176	PHE	2.1
1	F	652	ASN	2.1
1	E	595	GLU	2.1
1	F	87	HIS	2.1
1	F	189	TRP	2.1
1	F	467	ARG	2.1
1	F	88	PRO	2.0
1	F	420	GLN	2.0
1	F	489	THR	2.0
1	F	446	PHE	2.0
1	F	41	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

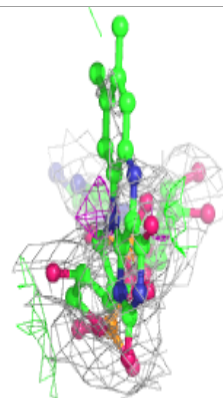
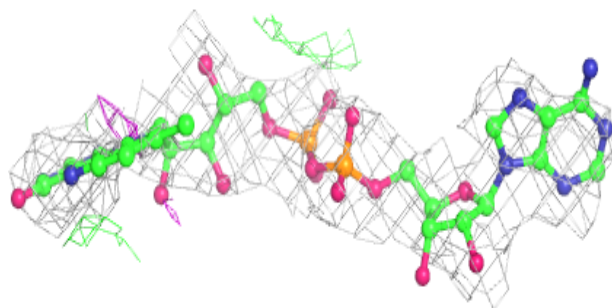
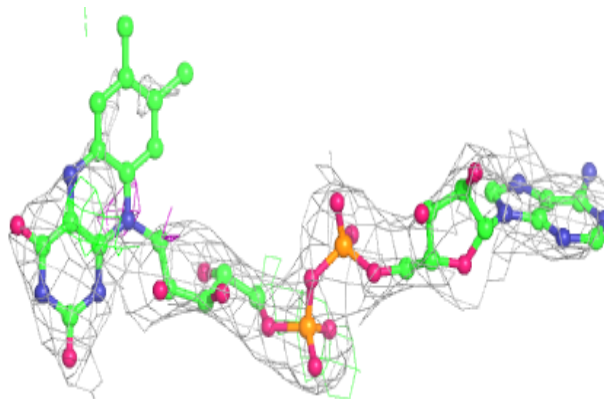
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	F	901	53/53	0.81	0.24	132,162,172,408	0
3	SO4	C	671	5/5	0.88	0.21	84,111,116,123	0
3	SO4	E	669	5/5	0.90	0.16	123,131,134,137	0
3	SO4	D	669	5/5	0.91	0.17	137,140,145,146	0
3	SO4	A	670	5/5	0.91	0.18	114,115,120,121	0
2	FAD	E	901	53/53	0.93	0.19	48,80,97,137	0
3	SO4	F	669	5/5	0.93	0.23	162,163,164,165	0
2	FAD	D	901	53/53	0.95	0.17	58,85,129,130	0
2	FAD	A	901	53/53	0.95	0.17	32,52,66,71	0
3	SO4	C	670	5/5	0.96	0.13	90,104,111,117	0
2	FAD	B	901	53/53	0.97	0.18	40,57,75,82	0
3	SO4	D	670	5/5	0.97	0.12	96,103,108,116	0
3	SO4	A	669	5/5	0.97	0.14	75,87,93,95	0
3	SO4	B	670	5/5	0.98	0.11	85,91,94,98	0
2	FAD	C	901	53/53	0.98	0.18	36,54,70,76	0
3	SO4	C	669	5/5	0.99	0.17	77,82,87,99	0
3	SO4	B	669	5/5	0.99	0.14	65,74,80,83	0

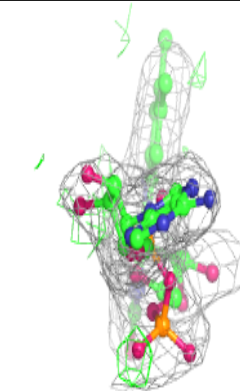
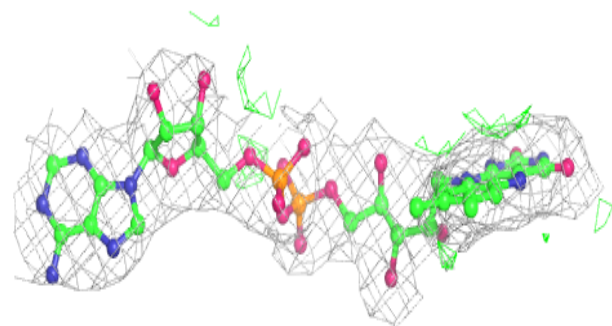
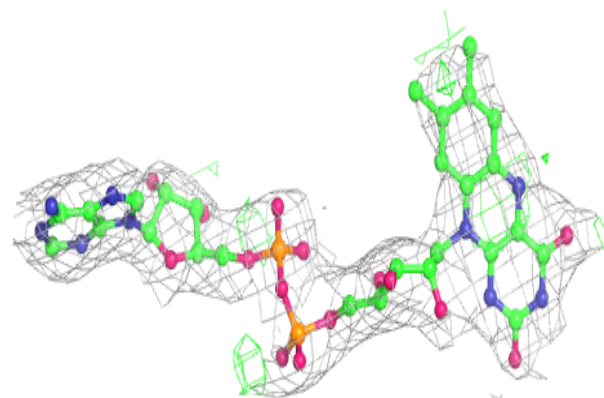
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

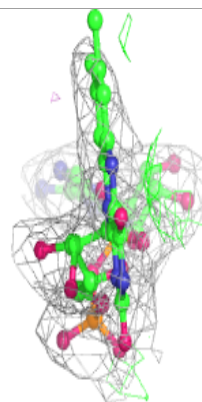
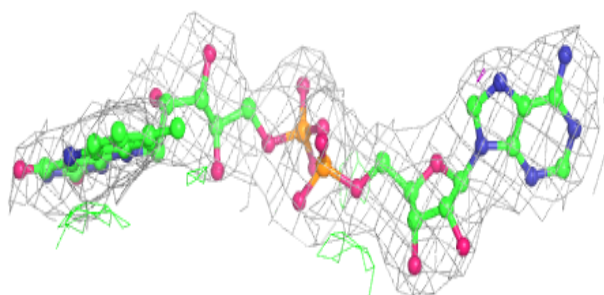
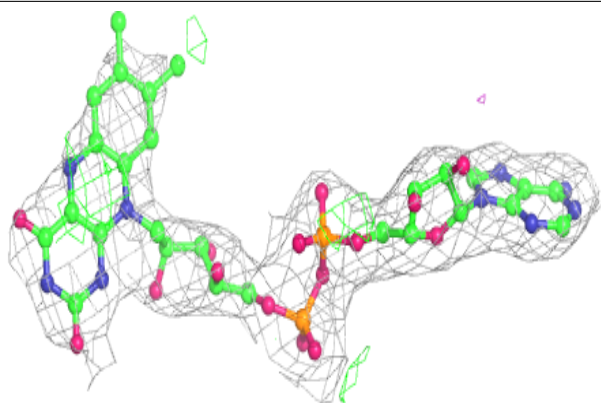
**Electron density around FAD E 901:**

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

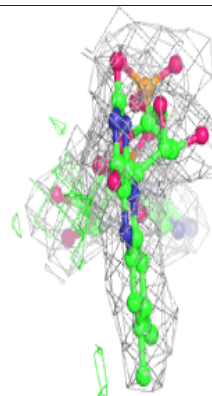
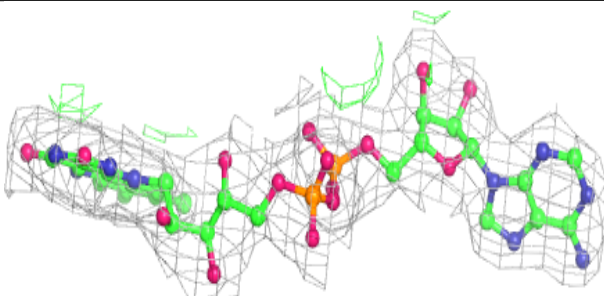
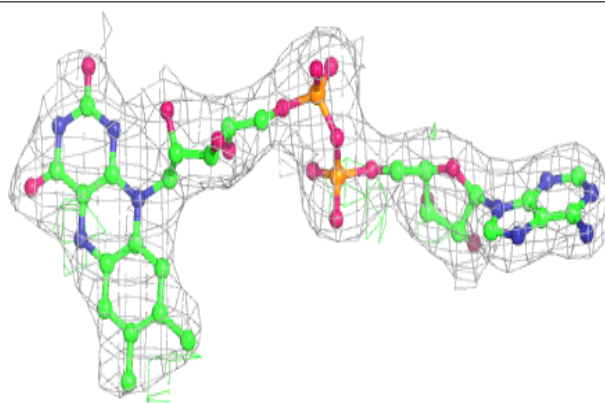


Electron density around FAD D 901:

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

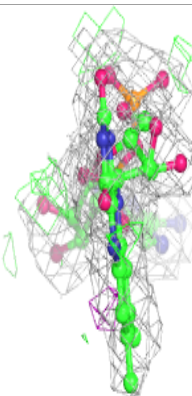
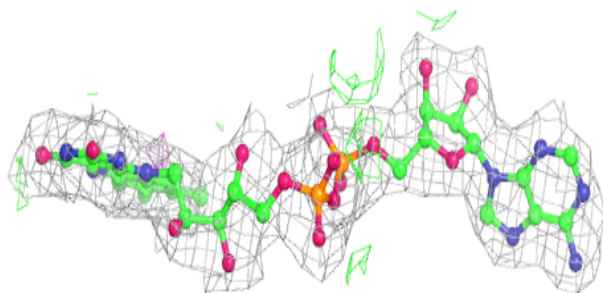
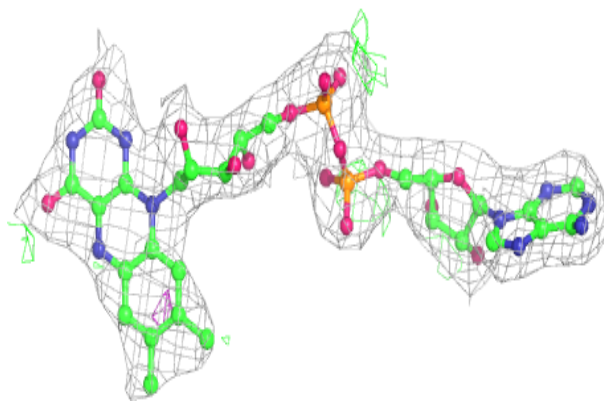
**Electron density around FAD A 901:**

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

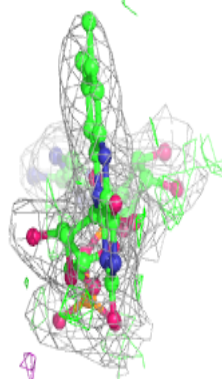
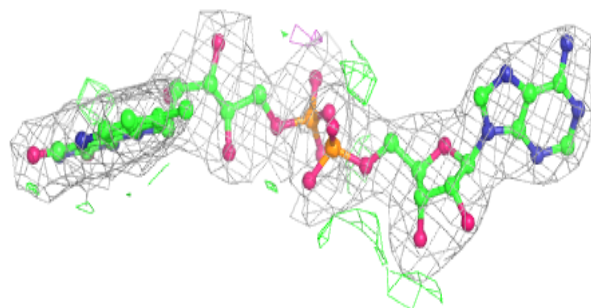
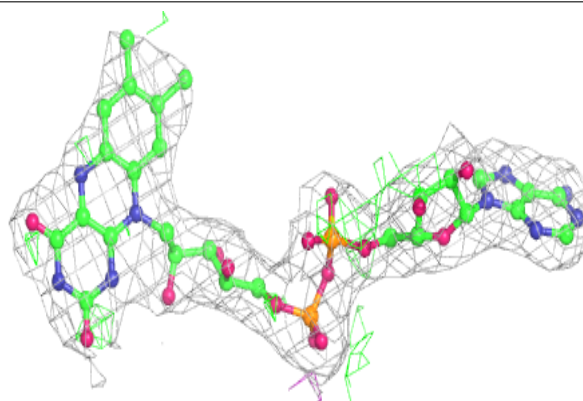


Electron density around FAD B 901:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.