



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:02 pm BST

PDB ID : 1DDO  
Title : REDUCED D-AMINO ACID OXIDASE FROM PIG KIDNEY IN COMPLEX  
WITH IMINO-TRP  
Authors : Todone, F.; Mattevi, A.  
Deposited on : 1997-01-16  
Resolution : 3.10 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](mailto: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.

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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

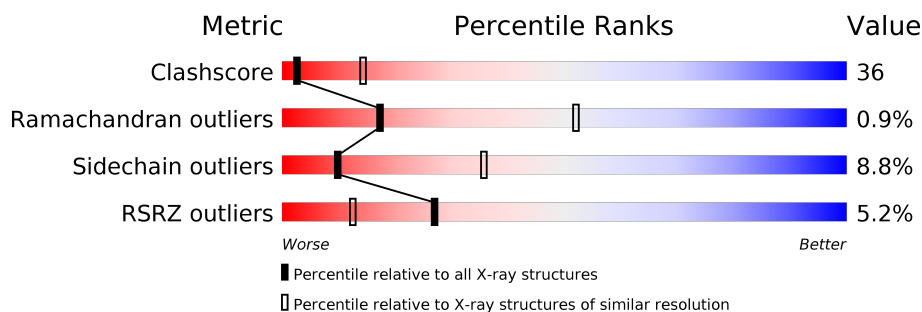
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.



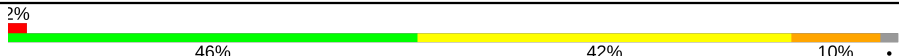
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	347	<div> <div>2%</div> <div>46%</div> <div>42%</div> <div>9%</div> <div>..</div> </div>
1	B	347	<div> <div>10%</div> <div>46%</div> <div>41%</div> <div>10%</div> <div>.</div> </div>
1	C	347	<div> <div>4%</div> <div>46%</div> <div>44%</div> <div>7%</div> <div>.</div> </div>
1	D	347	<div> <div>2%</div> <div>45%</div> <div>42%</div> <div>9%</div> <div>..</div> </div>
1	E	347	<div> <div>5%</div> <div>48%</div> <div>41%</div> <div>7%</div> <div>..</div> </div>
1	F	347	<div> <div>2%</div> <div>49%</div> <div>40%</div> <div>9%</div> <div>.</div> </div>
1	G	347	<div> <div>12%</div> <div>46%</div> <div>43%</div> <div>8%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	H	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DTR	E	350	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22441 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 D-AMINO ACID OXIDASE.

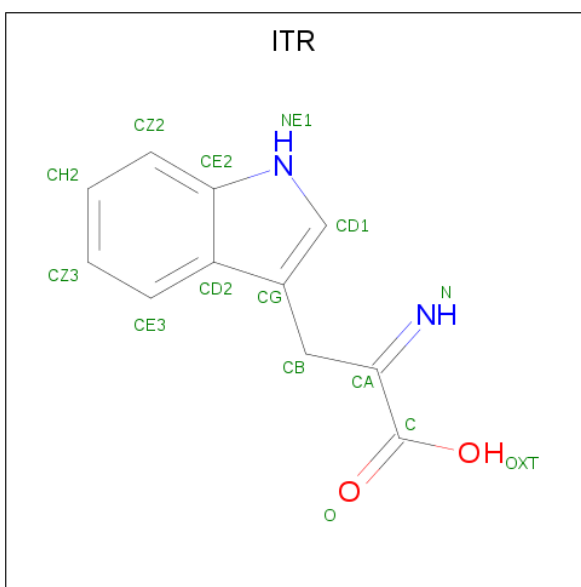
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	161	0	0
			2720	1749	473	489	9			
1	B	339	Total	C	N	O	S	190	0	0
			2720	1749	473	489	9			
1	C	339	Total	C	N	O	S	173	0	0
			2720	1749	473	489	9			
1	D	339	Total	C	N	O	S	131	0	0
			2720	1749	473	489	9			
1	E	339	Total	C	N	O	S	164	0	0
			2720	1749	473	489	9			
1	F	339	Total	C	N	O	S	154	0	0
			2720	1749	473	489	9			
1	G	339	Total	C	N	O	S	210	0	0
			2720	1749	473	489	9			
1	H	339	Total	C	N	O	S	166	0	0
			2720	1749	473	489	9			

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



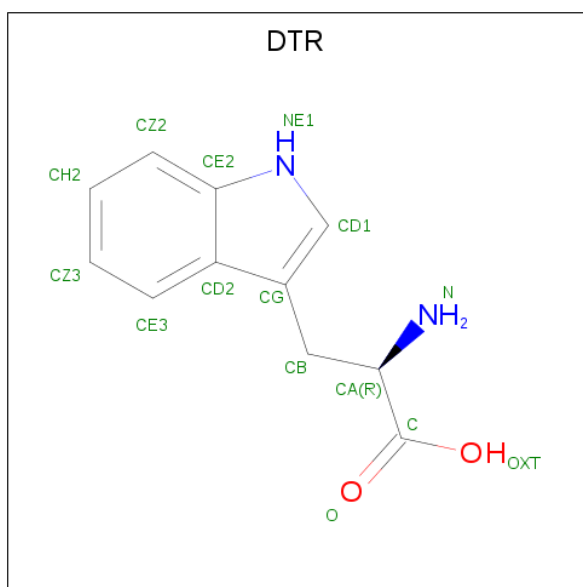
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G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

- Molecule 3 is IMINO-TRYPTOPHAN (three-letter code: ITR) (formula: C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	2	2		
3	B	1	Total	C	N	O	0	0
			15	11	2	2		
3	C	1	Total	C	N	O	0	0
			15	11	2	2		
3	D	1	Total	C	N	O	0	0
			15	11	2	2		
3	E	1	Total	C	N	O	0	0
			15	11	2	2		
3	F	1	Total	C	N	O	0	0
			15	11	2	2		
3	G	1	Total	C	N	O	0	0
			15	11	2	2		
3	H	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 4 is D-TRYPTOPHAN (three-letter code: DTR) (formula: C<sub>11</sub>H<sub>12</sub>N<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	E	1	Total	C	N	O	0	0
			15	11	2	2		
4	F	1	Total	C	N	O	0	0
			15	11	2	2		

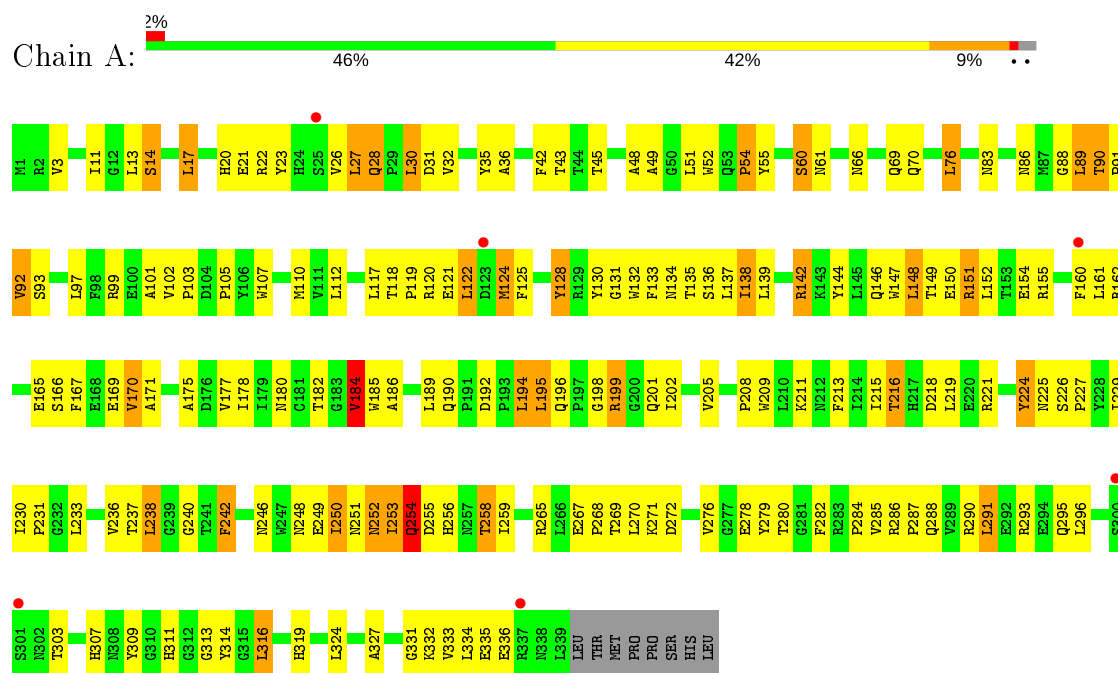
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	B	7	Total	O	0	0
			7	7		
5	C	12	Total	O	0	0
			12	12		
5	D	21	Total	O	0	0
			21	21		
5	E	16	Total	O	0	0
			16	16		
5	F	21	Total	O	0	0
			21	21		
5	G	3	Total	O	0	0
			3	3		
5	H	10	Total	O	0	0
			10	10		

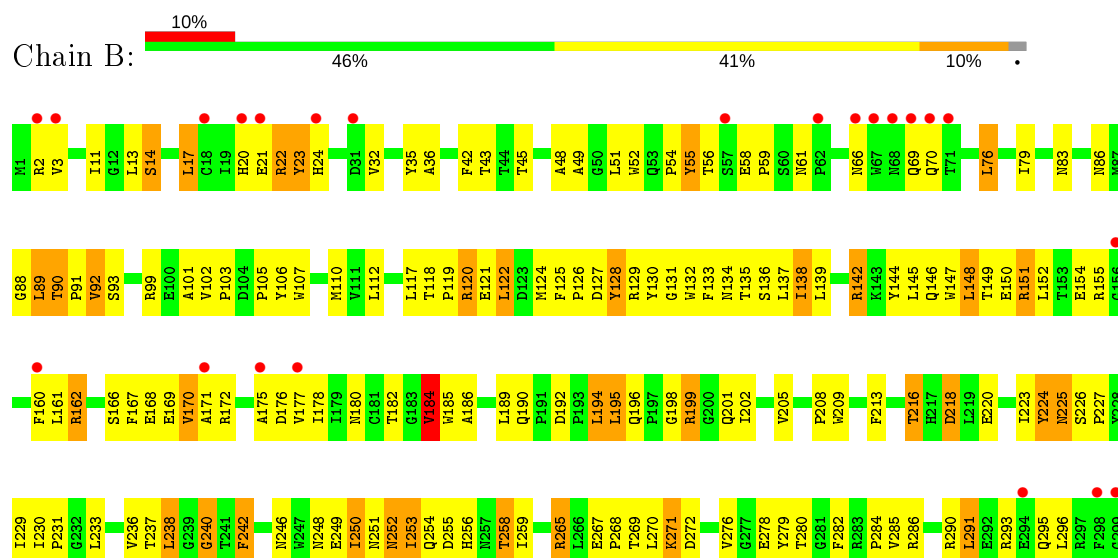
### 3 Residue-property plots

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.

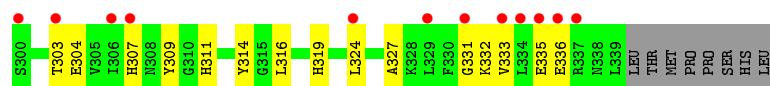
#### • Molecule 1: D-AMINO ACID OXIDASE



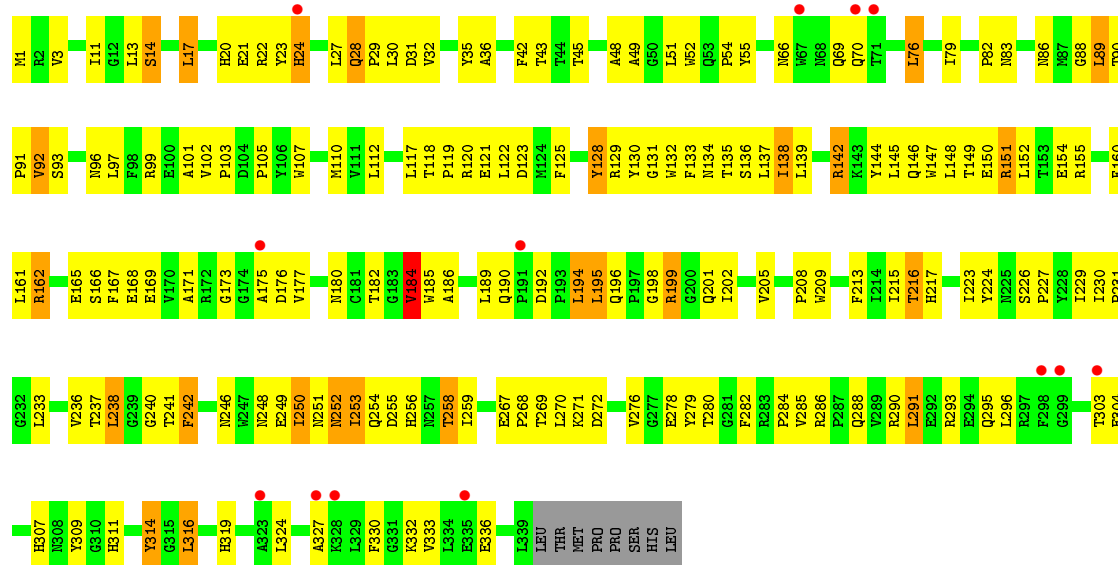
#### • Molecule 1: D-AMINO ACID OXIDASE



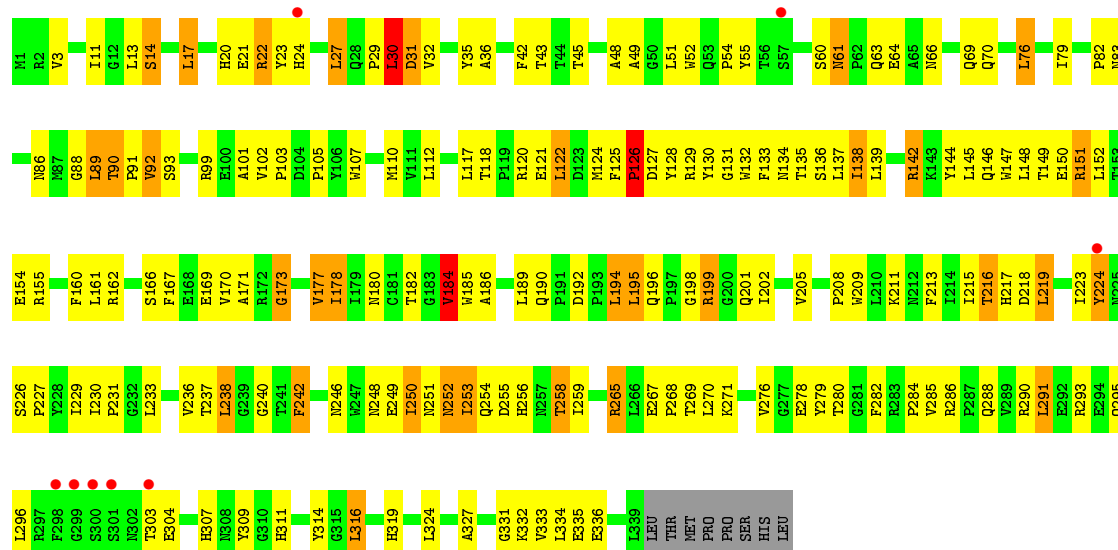




• Molecule 1: D-AMINO ACID OXIDASE

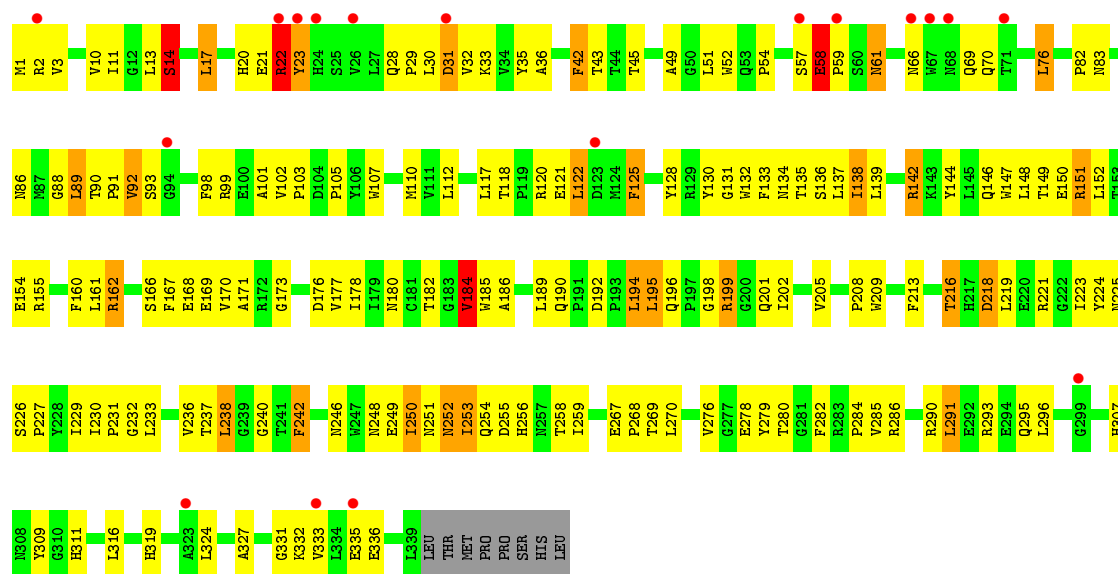


• Molecule 1: D-AMINO ACID OXIDASE

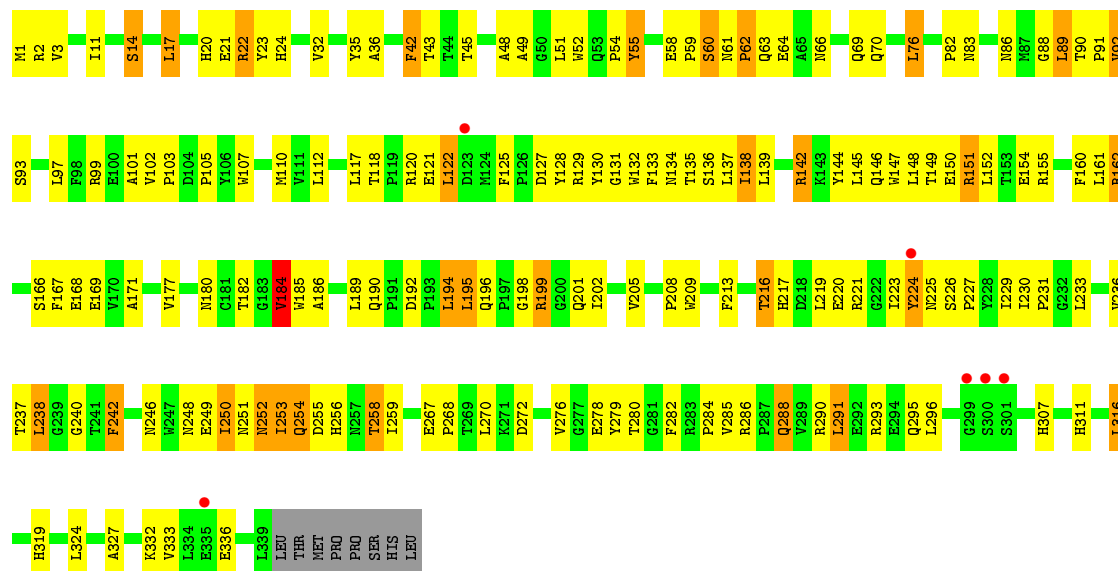
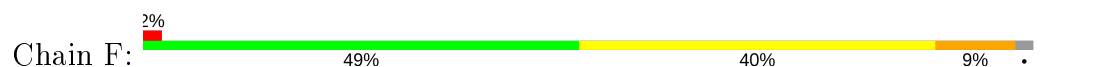


• Molecule 1: D-AMINO ACID OXIDASE

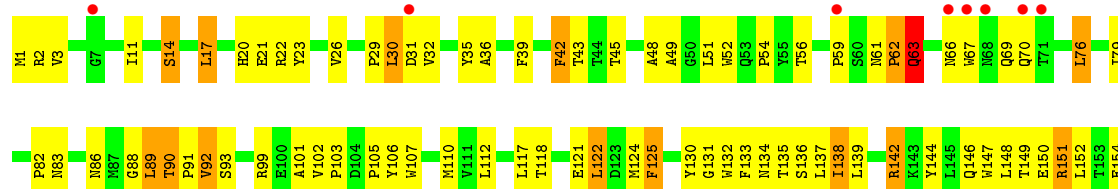


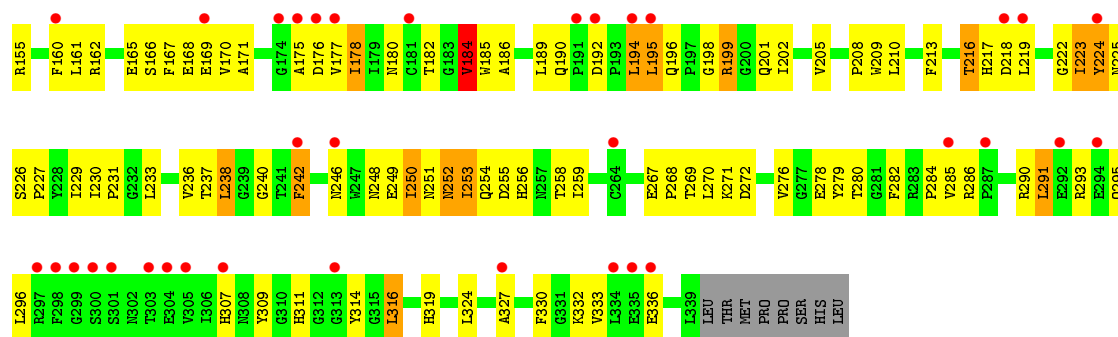


• Molecule 1: D-AMINO ACID OXIDASE

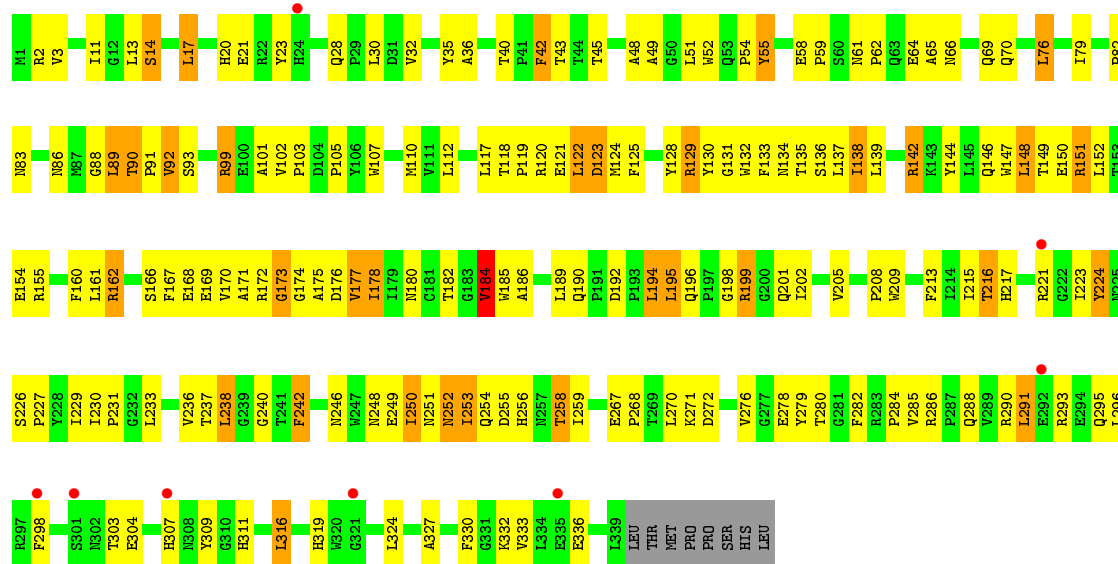


• Molecule 1: D-AMINO ACID OXIDASE





• Molecule 1: D-AMINO ACID OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	325.20 Å   137.10 Å   196.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.10 78.06 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (20.00-3.10) 98.0 (78.06-3.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.18 (at 3.13 Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, $R_{free}$	0.236 ,   0.250 0.235 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.4	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 120.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	22441	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DTR, ITR, 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	0.94	1/2796 (0.0%)	1.37	28/3808 (0.7%)
1	B	0.91	0/2796	1.34	27/3808 (0.7%)
1	C	0.90	0/2796	1.32	24/3808 (0.6%)
1	D	0.97	1/2796 (0.0%)	1.41	36/3808 (0.9%)
1	E	0.93	3/2796 (0.1%)	1.37	28/3808 (0.7%)
1	F	0.93	1/2796 (0.0%)	1.37	24/3808 (0.6%)
1	G	0.89	0/2796	1.34	21/3808 (0.6%)
1	H	0.92	2/2796 (0.1%)	1.34	24/3808 (0.6%)
All	All	0.92	8/22368 (0.0%)	1.36	212/30464 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	1	0
1	E	0	2
1	F	0	1
All	All	1	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	SER	CB-OG	8.68	1.53	1.42
1	E	23	TYR	CE1-CZ	-8.57	1.27	1.38
1	D	177	VAL	CB-CG1	-7.10	1.38	1.52
1	H	177	VAL	CB-CG1	-5.69	1.41	1.52
1	E	58	GLU	CG-CD	5.65	1.60	1.51
1	E	23	TYR	CD1-CE1	5.36	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	55	TYR	CD1-CE1	5.24	1.47	1.39
1	F	220	GLU	CD-OE2	-5.16	1.20	1.25

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	23	TYR	CG-CD1-CE1	-13.65	110.38	121.30
1	G	61	ASN	C-N-CD	-11.53	95.24	120.60
1	D	27	LEU	CA-CB-CG	10.98	140.55	115.30
1	C	194	LEU	CA-CB-CG	-8.93	94.75	115.30
1	D	194	LEU	CA-CB-CG	-8.93	94.75	115.30
1	E	194	LEU	CA-CB-CG	-8.93	94.77	115.30
1	A	194	LEU	CA-CB-CG	-8.93	94.77	115.30
1	B	194	LEU	CA-CB-CG	-8.93	94.77	115.30
1	F	194	LEU	CA-CB-CG	-8.92	94.77	115.30
1	H	194	LEU	CA-CB-CG	-8.92	94.79	115.30
1	G	194	LEU	CA-CB-CG	-8.92	94.79	115.30
1	E	23	TYR	CB-CG-CD1	-8.83	115.70	121.00
1	D	125	PHE	C-N-CD	-8.67	101.52	120.60
1	A	224	TYR	N-CA-C	8.29	133.38	111.00
1	E	22	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	G	286	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	D	286	ARG	NE-CZ-NH1	-7.88	116.36	120.30
1	E	286	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	C	286	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	H	286	ARG	NE-CZ-NH1	-7.83	116.39	120.30
1	F	286	ARG	NE-CZ-NH1	-7.76	116.42	120.30
1	A	286	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	B	286	ARG	NE-CZ-NH1	-7.74	116.43	120.30
1	A	92	VAL	CB-CA-C	-7.59	96.97	111.40
1	D	92	VAL	CB-CA-C	-7.58	96.99	111.40
1	F	92	VAL	CB-CA-C	-7.58	96.99	111.40
1	C	92	VAL	CB-CA-C	-7.58	97.00	111.40
1	H	92	VAL	CB-CA-C	-7.58	97.00	111.40
1	E	92	VAL	CB-CA-C	-7.57	97.01	111.40
1	B	92	VAL	CB-CA-C	-7.56	97.03	111.40
1	G	92	VAL	CB-CA-C	-7.56	97.03	111.40
1	E	221	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	A	254	GLN	CB-CA-C	-7.50	95.40	110.40
1	B	23	TYR	N-CA-C	7.29	130.69	111.00
1	E	162	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	D	30	LEU	CB-CG-CD2	-7.18	98.80	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	199	ARG	NE-CZ-NH1	-7.17	116.71	120.30
1	A	199	ARG	NE-CZ-NH1	-7.17	116.72	120.30
1	B	199	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	D	265	ARG	CG-CD-NE	-7.13	96.82	111.80
1	H	221	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	F	199	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	C	199	ARG	NE-CZ-NH1	-7.07	116.76	120.30
1	H	199	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	D	27	LEU	CB-CA-C	-7.05	96.81	110.20
1	F	162	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	E	199	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	E	218	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	D	199	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	C	195	LEU	CB-CG-CD1	-6.97	99.16	111.00
1	D	195	LEU	CB-CG-CD1	-6.96	99.16	111.00
1	A	195	LEU	CB-CG-CD1	-6.96	99.17	111.00
1	C	24	HIS	CB-CA-C	6.96	124.32	110.40
1	F	195	LEU	CB-CG-CD1	-6.95	99.19	111.00
1	H	195	LEU	CB-CG-CD1	-6.94	99.19	111.00
1	B	195	LEU	CB-CG-CD1	-6.94	99.21	111.00
1	E	195	LEU	CB-CG-CD1	-6.94	99.20	111.00
1	G	195	LEU	CB-CG-CD1	-6.94	99.21	111.00
1	F	2	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	D	127	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	A	128	TYR	CA-CB-CG	-6.79	100.50	113.40
1	D	90	THR	N-CA-CB	6.59	122.82	110.30
1	C	90	THR	N-CA-CB	6.58	122.81	110.30
1	E	90	THR	N-CA-CB	6.58	122.79	110.30
1	A	90	THR	N-CA-CB	6.57	122.78	110.30
1	G	90	THR	N-CA-CB	6.57	122.78	110.30
1	F	90	THR	N-CA-CB	6.57	122.78	110.30
1	B	90	THR	N-CA-CB	6.56	122.77	110.30
1	H	90	THR	N-CA-CB	6.56	122.76	110.30
1	G	62	PRO	N-CA-C	6.52	129.05	112.10
1	D	129	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	F	55	TYR	CB-CG-CD1	6.51	124.91	121.00
1	B	265	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	C	31	ASP	CB-CG-OD1	-6.33	112.60	118.30
1	F	184	VAL	CB-CA-C	-6.33	99.38	111.40
1	B	184	VAL	CB-CA-C	-6.32	99.39	111.40
1	A	184	VAL	CB-CA-C	-6.32	99.39	111.40
1	E	184	VAL	CB-CA-C	-6.32	99.40	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	184	VAL	CB-CA-C	-6.31	99.41	111.40
1	C	184	VAL	CB-CA-C	-6.30	99.42	111.40
1	D	184	VAL	CB-CA-C	-6.30	99.43	111.40
1	G	184	VAL	CB-CA-C	-6.30	99.44	111.40
1	H	162	ARG	CG-CD-NE	-6.21	98.75	111.80
1	A	225	ASN	C-N-CA	-6.21	106.17	121.70
1	E	162	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	225	ASN	C-N-CA	-6.15	106.33	121.70
1	D	23	TYR	N-CA-C	6.08	127.40	111.00
1	D	42	PHE	N-CA-C	6.02	127.26	111.00
1	C	42	PHE	N-CA-C	6.02	127.25	111.00
1	B	42	PHE	N-CA-C	6.02	127.24	111.00
1	G	42	PHE	N-CA-C	6.01	127.23	111.00
1	F	42	PHE	N-CA-C	6.01	127.22	111.00
1	A	42	PHE	N-CA-C	6.01	127.22	111.00
1	E	42	PHE	N-CA-C	6.00	127.21	111.00
1	H	42	PHE	N-CA-C	6.00	127.21	111.00
1	B	223	ILE	N-CA-C	6.00	127.19	111.00
1	H	122	LEU	CA-CB-CG	-5.95	101.61	115.30
1	F	122	LEU	CA-CB-CG	-5.95	101.62	115.30
1	C	122	LEU	CA-CB-CG	-5.94	101.63	115.30
1	E	122	LEU	CA-CB-CG	-5.94	101.63	115.30
1	C	162	ARG	CG-CD-NE	-5.94	99.33	111.80
1	A	122	LEU	CA-CB-CG	-5.94	101.65	115.30
1	G	122	LEU	CA-CB-CG	-5.94	101.65	115.30
1	F	14	SER	CB-CA-C	-5.93	98.83	110.10
1	B	122	LEU	CA-CB-CG	-5.93	101.66	115.30
1	D	122	LEU	CA-CB-CG	-5.93	101.66	115.30
1	B	14	SER	CB-CA-C	-5.93	98.84	110.10
1	E	14	SER	CB-CA-C	-5.92	98.85	110.10
1	A	14	SER	CB-CA-C	-5.92	98.85	110.10
1	G	14	SER	CB-CA-C	-5.92	98.85	110.10
1	D	14	SER	CB-CA-C	-5.91	98.87	110.10
1	C	14	SER	CB-CA-C	-5.91	98.88	110.10
1	H	14	SER	CB-CA-C	-5.90	98.88	110.10
1	H	202	ILE	CB-CA-C	-5.89	99.81	111.60
1	A	202	ILE	CB-CA-C	-5.88	99.84	111.60
1	F	202	ILE	CB-CA-C	-5.88	99.84	111.60
1	B	198	GLY	N-CA-C	-5.88	98.41	113.10
1	G	202	ILE	CB-CA-C	-5.87	99.86	111.60
1	C	198	GLY	N-CA-C	-5.87	98.42	113.10
1	C	202	ILE	CB-CA-C	-5.87	99.86	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	198	GLY	N-CA-C	-5.87	98.43	113.10
1	F	198	GLY	N-CA-C	-5.87	98.44	113.10
1	D	202	ILE	CB-CA-C	-5.86	99.88	111.60
1	H	198	GLY	N-CA-C	-5.86	98.45	113.10
1	E	198	GLY	N-CA-C	-5.86	98.45	113.10
1	B	202	ILE	CB-CA-C	-5.86	99.88	111.60
1	E	202	ILE	CB-CA-C	-5.85	99.89	111.60
1	A	198	GLY	N-CA-C	-5.85	98.47	113.10
1	D	198	GLY	N-CA-C	-5.85	98.48	113.10
1	D	129	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	D	64	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	A	27	LEU	CB-CG-CD2	-5.81	101.13	111.00
1	B	129	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	250	ILE	CB-CA-C	-5.75	100.10	111.60
1	F	250	ILE	CB-CA-C	-5.74	100.11	111.60
1	D	250	ILE	CB-CA-C	-5.74	100.12	111.60
1	H	250	ILE	CB-CA-C	-5.74	100.12	111.60
1	C	250	ILE	CB-CA-C	-5.74	100.12	111.60
1	E	250	ILE	CB-CA-C	-5.73	100.13	111.60
1	A	250	ILE	CB-CA-C	-5.73	100.14	111.60
1	G	250	ILE	CB-CA-C	-5.73	100.14	111.60
1	B	218	ASP	CB-CG-OD1	-5.72	113.15	118.30
1	F	127	ASP	CB-CA-C	5.72	121.83	110.40
1	C	199	ARG	NE-CZ-NH2	5.68	123.14	120.30
1	F	162	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	G	199	ARG	NE-CZ-NH2	5.67	123.13	120.30
1	B	199	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	F	199	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	199	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	H	199	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	D	199	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	125	PHE	CB-CA-C	-5.52	99.36	110.40
1	C	27	LEU	N-CA-C	-5.52	96.10	111.00
1	D	288	GLN	N-CA-C	-5.51	96.12	111.00
1	E	199	ARG	NE-CZ-NH2	5.51	123.06	120.30
1	A	271	LYS	O-C-N	5.49	131.49	122.70
1	F	129	ARG	CA-CB-CG	5.49	125.47	113.40
1	G	178	ILE	CG1-CB-CG2	5.48	123.46	111.40
1	C	314	TYR	CB-CG-CD2	5.47	124.28	121.00
1	B	162	ARG	N-CA-CB	-5.47	100.75	110.60
1	E	31	ASP	N-CA-CB	-5.45	100.80	110.60
1	D	219	LEU	CA-CB-CG	-5.44	102.78	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	316	LEU	CA-CB-CG	-5.43	102.81	115.30
1	D	129	ARG	NH1-CZ-NH2	5.42	125.36	119.40
1	E	316	LEU	CA-CB-CG	-5.41	102.86	115.30
1	A	316	LEU	CA-CB-CG	-5.40	102.87	115.30
1	D	316	LEU	CA-CB-CG	-5.40	102.87	115.30
1	G	316	LEU	CA-CB-CG	-5.40	102.89	115.30
1	F	316	LEU	CA-CB-CG	-5.40	102.89	115.30
1	H	316	LEU	CA-CB-CG	-5.39	102.90	115.30
1	C	316	LEU	CA-CB-CG	-5.39	102.91	115.30
1	D	126	PRO	C-N-CA	-5.36	108.31	121.70
1	B	170	VAL	C-N-CA	-5.35	108.33	121.70
1	A	128	TYR	CB-CG-CD1	-5.31	117.82	121.00
1	C	128	TYR	CA-CB-CG	-5.30	103.33	113.40
1	D	178	ILE	CG1-CB-CG2	5.29	123.05	111.40
1	H	178	ILE	N-CA-C	-5.28	96.73	111.00
1	H	288	GLN	N-CA-C	-5.28	96.73	111.00
1	E	125	PHE	N-CA-C	-5.28	96.75	111.00
1	C	149	THR	CA-CB-CG2	-5.21	105.10	112.40
1	H	177	VAL	CG1-CB-CG2	-5.21	102.56	110.90
1	D	149	THR	CA-CB-CG2	-5.21	105.11	112.40
1	F	149	THR	CA-CB-CG2	-5.20	105.12	112.40
1	E	149	THR	CA-CB-CG2	-5.19	105.14	112.40
1	H	149	THR	CA-CB-CG2	-5.18	105.15	112.40
1	G	149	THR	CA-CB-CG2	-5.17	105.16	112.40
1	A	149	THR	CA-CB-CG2	-5.16	105.17	112.40
1	B	149	THR	CA-CB-CG2	-5.16	105.18	112.40
1	D	31	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	C	120	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	D	129	ARG	CB-CA-C	-5.11	100.19	110.40
1	E	177	VAL	CB-CA-C	-5.08	101.74	111.40
1	H	120	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	170	VAL	CA-CB-CG1	-5.08	103.29	110.90
1	D	120	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	F	120	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	120	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	H	162	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	148	LEU	CB-CG-CD1	5.05	119.59	111.00
1	F	148	LEU	CB-CG-CD1	5.05	119.58	111.00
1	E	120	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	A	124	MET	CB-CG-SD	-5.04	97.28	112.40
1	E	148	LEU	CB-CG-CD1	5.03	119.55	111.00
1	C	148	LEU	CB-CG-CD1	5.03	119.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	148	LEU	CB-CG-CD1	5.03	119.55	111.00
1	A	148	LEU	CB-CG-CD1	5.02	119.54	111.00
1	D	173	GLY	N-CA-C	-5.02	100.54	113.10
1	G	63	GLN	N-CA-CB	-5.02	101.56	110.60
1	D	148	LEU	CB-CG-CD1	5.02	119.54	111.00
1	B	120	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	H	148	LEU	CB-CG-CD1	5.01	119.52	111.00
1	A	170	VAL	CB-CA-C	-5.01	101.89	111.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	23	TYR	CA

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	PRO	Mainchain
1	E	23	TYR	Sidechain
1	E	58	GLU	Sidechain
1	F	23	TYR	Sidechain

## 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	2720	0	2675	181	1
1	B	2720	0	2675	197	0
1	C	2720	0	2675	176	3
1	D	2720	0	2675	223	1
1	E	2720	0	2675	187	0
1	F	2720	0	2675	186	0
1	G	2720	0	2675	204	0
1	H	2720	0	2675	189	3
2	A	53	0	31	5	0
2	B	53	0	31	3	0
2	C	53	0	31	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	31	4	0
2	E	53	0	31	2	0
2	F	53	0	31	4	0
2	G	53	0	31	5	0
2	H	53	0	31	5	0
3	A	15	0	8	0	0
3	B	15	0	8	0	0
3	C	15	0	8	0	0
3	D	15	0	8	0	0
3	E	15	0	8	0	0
3	F	15	0	8	1	0
3	G	15	0	8	0	0
3	H	15	0	8	0	0
4	E	15	0	11	7	0
4	F	15	0	11	3	0
5	A	17	0	0	0	0
5	B	7	0	0	3	0
5	C	12	0	0	2	0
5	D	21	0	0	5	0
5	E	16	0	0	0	0
5	F	21	0	0	3	0
5	G	3	0	0	1	0
5	H	10	0	0	0	0
All	All	22441	0	21734	1493	4

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 36.

All (1493) 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:D:223:ILE:HG13	1:D:224:TYR:CE1	1.52	1.42
1:D:223:ILE:HG13	1:D:224:TYR:CD1	1.69	1.27
1:A:253:ILE:HG12	1:F:42:PHE:CD1	1.73	1.23
1:E:22:ARG:HG3	1:E:22:ARG:HH11	1.09	1.14
1:F:223:ILE:HG12	1:F:224:TYR:CD1	1.85	1.11
1:D:216:THR:HG22	1:D:226:SER:HB3	1.33	1.11
1:B:201:GLN:HG3	1:B:280:THR:HG22	1.32	1.10
1:F:201:GLN:HG3	1:F:280:THR:HG22	1.32	1.10
1:B:216:THR:HG22	1:B:226:SER:HB3	1.33	1.10
1:A:201:GLN:HG3	1:A:280:THR:HG22	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201:GLN:HG3	1:C:280:THR:HG22	1.32	1.09
1:E:216:THR:HG22	1:E:226:SER:HB3	1.33	1.09
1:F:216:THR:HG22	1:F:226:SER:HB3	1.33	1.08
1:E:201:GLN:HG3	1:E:280:THR:HG22	1.32	1.08
1:H:216:THR:HG22	1:H:226:SER:HB3	1.33	1.08
1:C:216:THR:HG22	1:C:226:SER:HB3	1.33	1.08
1:D:27:LEU:HD12	1:D:30:LEU:HB2	1.13	1.08
1:D:201:GLN:HG3	1:D:280:THR:HG22	1.32	1.08
1:A:216:THR:HG22	1:A:226:SER:HB3	1.33	1.08
1:D:171:ALA:HB1	1:D:303:THR:HG21	1.36	1.08
1:G:201:GLN:HG3	1:G:280:THR:HG22	1.32	1.07
1:G:216:THR:HG22	1:G:226:SER:HB3	1.33	1.06
1:D:223:ILE:CG1	1:D:224:TYR:CE1	2.37	1.06
1:H:201:GLN:HG3	1:H:280:THR:HG22	1.32	1.05
1:D:216:THR:CG2	1:D:226:SER:HB3	1.88	1.04
1:E:256:HIS:ND1	1:E:278:GLU:OE2	1.91	1.04
1:G:216:THR:CG2	1:G:226:SER:HB3	1.88	1.04
1:D:256:HIS:ND1	1:D:278:GLU:OE2	1.91	1.03
1:G:256:HIS:ND1	1:G:278:GLU:OE2	1.91	1.03
1:H:216:THR:CG2	1:H:226:SER:HB3	1.88	1.03
1:A:256:HIS:ND1	1:A:278:GLU:OE2	1.91	1.03
1:C:69:GLN:HB2	1:C:110:MET:HE3	1.39	1.03
1:F:216:THR:CG2	1:F:226:SER:HB3	1.88	1.03
1:E:216:THR:CG2	1:E:226:SER:HB3	1.88	1.02
1:F:256:HIS:ND1	1:F:278:GLU:OE2	1.91	1.02
1:B:256:HIS:ND1	1:B:278:GLU:OE2	1.91	1.02
1:B:216:THR:CG2	1:B:226:SER:HB3	1.88	1.02
1:H:256:HIS:ND1	1:H:278:GLU:OE2	1.91	1.02
1:C:256:HIS:ND1	1:C:278:GLU:OE2	1.91	1.02
1:A:216:THR:CG2	1:A:226:SER:HB3	1.88	1.01
1:D:253:ILE:HG12	1:G:42:PHE:CD1	1.95	1.01
1:C:216:THR:CG2	1:C:226:SER:HB3	1.88	1.01
1:G:69:GLN:HB2	1:G:110:MET:HE3	1.42	0.98
1:H:69:GLN:HB2	1:H:110:MET:HE3	1.45	0.98
1:A:69:GLN:HB2	1:A:110:MET:HE3	1.42	0.97
1:D:223:ILE:HG13	1:D:224:TYR:HE1	1.25	0.97
1:B:69:GLN:HB2	1:B:110:MET:HE2	1.45	0.96
1:B:253:ILE:HG12	1:E:42:PHE:CD1	2.00	0.95
1:D:69:GLN:HB2	1:D:110:MET:HE3	1.47	0.95
1:G:30:LEU:HD12	1:G:31:ASP:N	1.81	0.94
1:E:69:GLN:HB2	1:E:110:MET:HE3	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ASN:HD22	1:D:63:GLN:HE21	1.12	0.94
1:D:22:ARG:O	1:D:22:ARG:HD2	1.67	0.94
1:D:223:ILE:CG1	1:D:224:TYR:HE1	1.78	0.93
1:G:62:PRO:HG2	1:G:63:GLN:HG3	1.52	0.92
1:B:171:ALA:HB1	1:B:303:THR:HG21	1.51	0.92
1:B:216:THR:HG22	1:B:226:SER:CB	2.01	0.90
1:H:121:GLU:HA	1:H:124:MET:HE2	1.49	0.90
1:H:216:THR:HG22	1:H:226:SER:CB	2.02	0.90
1:C:216:THR:HG22	1:C:226:SER:CB	2.01	0.90
1:D:69:GLN:HB2	1:D:110:MET:CE	2.02	0.90
1:D:216:THR:HG22	1:D:226:SER:CB	2.02	0.90
1:A:253:ILE:HG12	1:F:42:PHE:CE1	2.07	0.90
1:F:61:ASN:OD1	1:F:63:GLN:HG3	1.71	0.90
1:G:69:GLN:HB2	1:G:110:MET:CE	2.02	0.90
1:F:69:GLN:HB2	1:F:110:MET:CE	2.02	0.89
1:G:216:THR:HG22	1:G:226:SER:CB	2.02	0.89
1:E:69:GLN:HB2	1:E:110:MET:CE	2.02	0.89
1:E:216:THR:HG22	1:E:226:SER:CB	2.02	0.89
1:E:2:ARG:HD3	4:E:350:DTR:CD2	2.03	0.89
1:H:69:GLN:HB2	1:H:110:MET:CE	2.02	0.89
1:A:69:GLN:HB2	1:A:110:MET:CE	2.02	0.89
1:A:216:THR:HG22	1:A:226:SER:CB	2.02	0.89
1:C:253:ILE:HG12	1:H:42:PHE:CD1	2.07	0.88
1:F:216:THR:HG22	1:F:226:SER:CB	2.02	0.88
1:D:27:LEU:CD1	1:D:30:LEU:HB2	2.02	0.88
1:C:69:GLN:HB2	1:C:110:MET:CE	2.02	0.88
1:F:69:GLN:HB2	1:F:110:MET:HE3	1.54	0.88
1:B:69:GLN:HB2	1:B:110:MET:CE	2.02	0.88
1:G:171:ALA:HA	1:G:175:ALA:HB3	1.56	0.87
1:G:59:PRO:HG3	1:G:106:TYR:CZ	2.09	0.87
1:F:223:ILE:HG12	1:F:224:TYR:HD1	1.40	0.87
1:D:61:ASN:HD22	1:D:63:GLN:NE2	1.73	0.86
1:A:253:ILE:CG1	1:F:42:PHE:CD1	2.57	0.86
1:B:2:ARG:O	1:B:176:ASP:HB2	1.76	0.86
1:B:250:ILE:CD1	1:E:250:ILE:HD13	2.05	0.85
1:E:2:ARG:O	1:E:176:ASP:HB2	1.77	0.85
1:H:168:GLU:HA	1:H:171:ALA:HB3	1.60	0.84
1:D:90:THR:HG22	5:D:369:HOH:O	1.78	0.84
1:A:27:LEU:HD11	1:A:334:LEU:HD11	1.60	0.83
1:H:2:ARG:NH1	1:H:173:GLY:O	2.12	0.83
1:H:168:GLU:O	1:H:172:ARG:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:216:THR:HB	1:G:227:PRO:O	1.79	0.83
1:F:216:THR:HB	1:F:227:PRO:O	1.79	0.82
1:A:216:THR:HB	1:A:227:PRO:O	1.79	0.82
1:H:216:THR:HB	1:H:227:PRO:O	1.79	0.82
1:D:216:THR:HB	1:D:227:PRO:O	1.79	0.82
1:D:223:ILE:HG23	1:D:224:TYR:CD1	2.14	0.82
1:A:287:PRO:HB2	1:A:288:GLN:NE2	1.96	0.81
1:F:60:SER:HB3	1:F:288:GLN:HG2	1.63	0.81
1:E:216:THR:HB	1:E:227:PRO:O	1.79	0.81
1:C:216:THR:HB	1:C:227:PRO:O	1.79	0.81
1:D:171:ALA:CB	1:D:303:THR:HG21	2.10	0.81
1:B:216:THR:HB	1:B:227:PRO:O	1.79	0.80
1:G:201:GLN:HE22	1:G:252:ASN:H	1.29	0.80
1:C:201:GLN:HE22	1:C:252:ASN:H	1.29	0.80
1:H:201:GLN:HE22	1:H:252:ASN:H	1.29	0.80
1:B:59:PRO:HB2	1:B:61:ASN:O	1.82	0.80
1:A:201:GLN:HE22	1:A:252:ASN:H	1.29	0.79
1:B:201:GLN:HE22	1:B:252:ASN:H	1.29	0.79
1:C:268:PRO:O	1:C:271:LYS:HB3	1.83	0.79
1:D:223:ILE:CG1	1:D:224:TYR:CD1	2.59	0.79
1:E:201:GLN:HE22	1:E:252:ASN:H	1.29	0.79
1:G:62:PRO:HG2	1:G:63:GLN:CG	2.12	0.79
1:B:250:ILE:HD13	1:E:250:ILE:HD13	1.64	0.79
1:B:218:ASP:OD1	1:B:220:GLU:HG2	1.83	0.79
1:D:61:ASN:HB2	1:D:63:GLN:HG3	1.65	0.79
1:H:167:PHE:O	1:H:171:ALA:N	2.15	0.79
1:B:118:THR:HG23	1:B:121:GLU:OE1	1.83	0.79
1:C:66:ASN:O	1:C:70:GLN:HG3	1.83	0.79
1:D:30:LEU:HD12	1:D:31:ASP:N	1.98	0.79
1:H:66:ASN:O	1:H:70:GLN:HG3	1.83	0.79
1:D:201:GLN:HE22	1:D:252:ASN:H	1.29	0.78
1:A:66:ASN:O	1:A:70:GLN:HG3	1.83	0.78
1:C:1:MET:HB2	1:C:176:ASP:OD2	1.83	0.78
1:E:118:THR:HG23	1:E:121:GLU:OE1	1.83	0.78
1:E:66:ASN:O	1:E:70:GLN:HG3	1.83	0.78
1:F:118:THR:HG23	1:F:121:GLU:OE1	1.83	0.78
1:A:118:THR:HG23	1:A:121:GLU:OE1	1.83	0.78
1:D:118:THR:HG23	1:D:121:GLU:OE1	1.83	0.78
1:D:66:ASN:O	1:D:70:GLN:HG3	1.83	0.78
1:D:30:LEU:HD12	1:D:30:LEU:C	2.04	0.78
1:F:201:GLN:HE22	1:F:252:ASN:H	1.29	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:ASN:O	1:F:70:GLN:HG3	1.83	0.78
1:H:118:THR:HG23	1:H:121:GLU:OE1	1.83	0.78
1:A:250:ILE:CD1	1:F:250:ILE:HD13	2.14	0.78
1:F:293:ARG:HH22	1:F:336:GLU:CD	1.88	0.78
1:B:251:ASN:OD1	1:B:280:THR:HG23	1.84	0.77
1:B:66:ASN:O	1:B:70:GLN:HG3	1.83	0.77
1:F:251:ASN:OD1	1:F:280:THR:HG23	1.84	0.77
1:C:253:ILE:HG12	1:H:42:PHE:CE1	2.18	0.77
1:G:118:THR:HG23	1:G:121:GLU:OE1	1.83	0.77
1:G:66:ASN:O	1:G:70:GLN:HG3	1.83	0.77
1:H:293:ARG:HH22	1:H:336:GLU:CD	1.88	0.77
1:C:251:ASN:OD1	1:C:280:THR:HG23	1.84	0.77
1:D:293:ARG:HH22	1:D:336:GLU:CD	1.88	0.77
1:G:251:ASN:OD1	1:G:280:THR:HG23	1.84	0.77
1:E:293:ARG:HH22	1:E:336:GLU:CD	1.88	0.77
1:A:251:ASN:OD1	1:A:280:THR:HG23	1.84	0.77
1:D:251:ASN:OD1	1:D:280:THR:HG23	1.84	0.77
1:G:293:ARG:HH22	1:G:336:GLU:CD	1.88	0.77
1:H:251:ASN:OD1	1:H:280:THR:HG23	1.84	0.77
1:C:118:THR:HG23	1:C:121:GLU:OE1	1.83	0.77
1:C:23:TYR:CE2	1:C:330:PHE:HD2	2.03	0.77
1:E:251:ASN:OD1	1:E:280:THR:HG23	1.84	0.77
1:A:293:ARG:HH22	1:A:336:GLU:CD	1.88	0.76
1:C:293:ARG:HH22	1:C:336:GLU:CD	1.88	0.76
1:A:250:ILE:HD11	1:F:250:ILE:HD13	1.67	0.76
1:B:293:ARG:HH22	1:B:336:GLU:CD	1.88	0.76
1:C:105:PRO:HD3	1:C:132:TRP:CZ2	2.21	0.76
1:D:105:PRO:HD3	1:D:132:TRP:CZ2	2.21	0.76
1:F:20:HIS:ND1	1:F:155:ARG:NH1	2.34	0.76
1:F:58:GLU:HB3	1:F:59:PRO:HD2	1.67	0.76
1:H:121:GLU:HA	1:H:124:MET:CE	2.15	0.76
1:B:20:HIS:ND1	1:B:155:ARG:NH1	2.34	0.76
1:F:105:PRO:HD3	1:F:132:TRP:CZ2	2.21	0.76
1:B:105:PRO:HD3	1:B:132:TRP:CZ2	2.21	0.75
1:B:250:ILE:HD11	1:E:250:ILE:CD1	2.16	0.75
1:G:20:HIS:ND1	1:G:155:ARG:NH1	2.34	0.75
1:D:20:HIS:ND1	1:D:155:ARG:NH1	2.34	0.75
1:E:105:PRO:HD3	1:E:132:TRP:CZ2	2.21	0.75
1:E:22:ARG:HG3	1:E:22:ARG:NH1	1.87	0.75
1:F:223:ILE:HG23	1:F:224:TYR:CD1	2.21	0.75
1:E:20:HIS:ND1	1:E:155:ARG:NH1	2.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ILE:CD1	1:E:250:ILE:CD1	2.64	0.75
1:G:105:PRO:HD3	1:G:132:TRP:CZ2	2.21	0.75
1:H:105:PRO:HD3	1:H:132:TRP:CZ2	2.21	0.75
1:A:27:LEU:HD11	1:A:334:LEU:CD1	2.17	0.74
1:A:27:LEU:HD12	1:A:30:LEU:HD22	1.69	0.74
1:A:20:HIS:ND1	1:A:155:ARG:NH1	2.34	0.74
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.21	0.74
1:H:20:HIS:ND1	1:H:155:ARG:NH1	2.34	0.74
1:C:55:TYR:HE1	1:C:314:TYR:CD1	2.06	0.74
1:C:20:HIS:ND1	1:C:155:ARG:NH1	2.34	0.74
1:H:58:GLU:CG	1:H:59:PRO:HD2	2.17	0.74
1:H:253:ILE:HG22	1:H:254:GLN:N	2.03	0.73
1:B:253:ILE:HG22	1:B:254:GLN:N	2.02	0.73
1:G:223:ILE:HB	1:G:224:TYR:CD1	2.24	0.73
4:F:350:DTR:H	4:F:350:DTR:CE3	2.01	0.73
1:D:223:ILE:C	1:D:224:TYR:HD1	1.93	0.72
1:E:253:ILE:HG22	1:E:254:GLN:N	2.04	0.72
1:H:224:TYR:HB2	1:H:242:PHE:HD2	1.54	0.72
1:D:102:VAL:HG13	1:D:103:PRO:HD2	1.72	0.72
1:D:121:GLU:OE2	5:D:357:HOH:O	2.06	0.72
1:E:218:ASP:HB2	1:E:226:SER:OG	1.90	0.72
1:F:102:VAL:HG13	1:F:103:PRO:HD2	1.72	0.72
1:C:255:ASP:O	1:C:259:ILE:HG13	1.90	0.71
1:G:201:GLN:CG	1:G:280:THR:HG22	2.18	0.71
1:C:69:GLN:CB	1:C:110:MET:HE3	2.19	0.71
1:B:128:TYR:N	1:B:128:TYR:CD1	2.55	0.71
1:C:201:GLN:CG	1:C:280:THR:HG22	2.18	0.71
1:D:255:ASP:O	1:D:259:ILE:HG13	1.90	0.71
1:D:291:LEU:HA	1:D:307:HIS:O	1.91	0.71
1:G:291:LEU:HA	1:G:307:HIS:O	1.91	0.71
1:G:63:GLN:O	1:G:67:TRP:N	2.14	0.71
1:F:223:ILE:HG12	1:F:224:TYR:CE1	2.26	0.71
1:A:201:GLN:CG	1:A:280:THR:HG22	2.18	0.71
1:A:255:ASP:O	1:A:259:ILE:HG13	1.90	0.70
1:C:102:VAL:HG13	1:C:103:PRO:HD2	1.72	0.70
1:F:255:ASP:O	1:F:259:ILE:HG13	1.90	0.70
1:H:255:ASP:O	1:H:259:ILE:HG13	1.90	0.70
1:B:102:VAL:HG13	1:B:103:PRO:HD2	1.72	0.70
1:E:255:ASP:O	1:E:259:ILE:HG13	1.90	0.70
1:F:201:GLN:CG	1:F:280:THR:HG22	2.18	0.70
1:B:255:ASP:O	1:B:259:ILE:HG13	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:291:LEU:HA	1:B:307:HIS:O	1.91	0.70
1:H:102:VAL:HG13	1:H:103:PRO:HD2	1.72	0.70
1:F:291:LEU:HA	1:F:307:HIS:O	1.91	0.70
1:G:255:ASP:O	1:G:259:ILE:HG13	1.90	0.70
1:H:291:LEU:HA	1:H:307:HIS:O	1.91	0.70
1:E:102:VAL:HG13	1:E:103:PRO:HD2	1.72	0.70
1:C:55:TYR:HE1	1:C:314:TYR:CE1	2.09	0.70
1:G:102:VAL:HG13	1:G:103:PRO:HD2	1.72	0.70
1:G:224:TYR:HB2	1:G:242:PHE:HB2	1.73	0.70
1:A:102:VAL:HG13	1:A:103:PRO:HD2	1.72	0.70
1:C:291:LEU:HA	1:C:307:HIS:O	1.91	0.70
1:A:268:PRO:HB2	1:E:82:PRO:HA	1.72	0.70
1:H:93:SER:OG	1:H:135:THR:HG23	1.92	0.70
1:E:291:LEU:HA	1:E:307:HIS:O	1.91	0.69
1:F:223:ILE:HG23	1:F:224:TYR:HD1	1.55	0.69
1:G:92:VAL:HG21	1:G:138:ILE:HG13	1.74	0.69
1:A:93:SER:OG	1:A:135:THR:HG23	1.92	0.69
1:A:92:VAL:HG21	1:A:138:ILE:HG13	1.74	0.69
1:D:211:LYS:O	5:D:370:HOH:O	2.09	0.69
1:A:291:LEU:HA	1:A:307:HIS:O	1.91	0.69
1:C:92:VAL:HG21	1:C:138:ILE:HG13	1.74	0.69
1:F:93:SER:OG	1:F:135:THR:HG23	1.92	0.69
1:G:93:SER:OG	1:G:135:THR:HG23	1.92	0.69
1:E:92:VAL:HG21	1:E:138:ILE:HG13	1.74	0.69
1:A:250:ILE:HD11	1:F:250:ILE:CD1	2.22	0.69
1:D:269:THR:C	1:D:271:LYS:H	1.96	0.69
1:H:58:GLU:HG3	1:H:59:PRO:CD	2.23	0.69
1:B:171:ALA:CB	1:B:303:THR:HG21	2.21	0.69
1:G:224:TYR:CD1	1:G:224:TYR:N	2.59	0.69
1:B:201:GLN:CG	1:B:280:THR:HG22	2.18	0.69
1:D:93:SER:OG	1:D:135:THR:HG23	1.92	0.69
1:F:92:VAL:HG21	1:F:138:ILE:HG13	1.74	0.68
1:B:93:SER:OG	1:B:135:THR:HG23	1.92	0.68
1:D:223:ILE:HG23	1:D:224:TYR:HD1	1.56	0.68
1:B:55:TYR:HE1	1:B:314:TYR:CD1	2.10	0.68
1:E:93:SER:OG	1:E:135:THR:HG23	1.92	0.68
1:B:92:VAL:HG21	1:B:138:ILE:HG13	1.74	0.68
1:C:93:SER:OG	1:C:135:THR:HG23	1.92	0.68
1:A:253:ILE:HG22	1:A:254:GLN:N	2.06	0.68
1:C:216:THR:HG21	1:C:226:SER:HB3	1.76	0.68
1:D:92:VAL:HG21	1:D:138:ILE:HG13	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:92:VAL:HG21	1:H:138:ILE:HG13	1.74	0.68
1:B:199:ARG:HH22	1:B:201:GLN:NE2	1.92	0.68
1:B:216:THR:HG21	1:B:226:SER:HB3	1.76	0.68
1:C:199:ARG:HH22	1:C:201:GLN:NE2	1.92	0.68
1:D:61:ASN:HB2	1:D:63:GLN:CG	2.24	0.68
1:H:23:TYR:O	1:H:30:LEU:HD22	1.93	0.68
1:E:216:THR:HG21	1:E:226:SER:HB3	1.76	0.68
1:H:199:ARG:HH22	1:H:201:GLN:NE2	1.92	0.67
1:B:224:TYR:HB2	1:B:242:PHE:HB2	1.75	0.67
1:E:295:GLN:O	1:E:296:LEU:HD23	1.95	0.67
1:H:295:GLN:O	1:H:296:LEU:HD23	1.95	0.67
1:G:223:ILE:CG2	1:G:224:TYR:CE1	2.77	0.67
1:C:82:PRO:HA	1:G:268:PRO:HB2	1.76	0.67
1:H:151:ARG:NH2	1:H:154:GLU:OE2	2.28	0.67
1:H:199:ARG:HH22	1:H:201:GLN:HE21	1.43	0.67
1:E:199:ARG:HH22	1:E:201:GLN:HE21	1.43	0.67
1:F:184:VAL:HG13	1:F:284:PRO:HA	1.77	0.67
1:G:224:TYR:HD1	1:G:224:TYR:N	1.93	0.67
1:D:199:ARG:HH22	1:D:201:GLN:HE21	1.43	0.67
1:E:184:VAL:HG13	1:E:284:PRO:HA	1.77	0.67
1:D:199:ARG:HH22	1:D:201:GLN:NE2	1.92	0.67
1:E:201:GLN:CG	1:E:280:THR:HG22	2.18	0.67
1:F:61:ASN:OD1	1:F:62:PRO:N	2.28	0.67
1:H:121:GLU:O	1:H:124:MET:HB2	1.95	0.67
1:C:201:GLN:NE2	1:C:252:ASN:H	1.93	0.67
1:C:295:GLN:O	1:C:296:LEU:HD23	1.95	0.67
1:F:293:ARG:NH2	1:F:336:GLU:OE1	2.28	0.67
1:G:293:ARG:NH2	1:G:336:GLU:OE1	2.28	0.67
1:A:151:ARG:NH2	1:A:154:GLU:OE2	2.28	0.67
1:A:36:ALA:O	1:A:161:LEU:HD12	1.95	0.67
1:B:201:GLN:NE2	1:B:252:ASN:H	1.93	0.67
1:B:256:HIS:HD1	1:B:278:GLU:CD	1.97	0.67
1:B:184:VAL:HG13	1:B:284:PRO:HA	1.77	0.67
1:B:293:ARG:NH2	1:B:336:GLU:OE1	2.28	0.67
1:G:199:ARG:HH22	1:G:201:GLN:HE21	1.43	0.67
1:A:201:GLN:NE2	1:A:252:ASN:H	1.93	0.66
1:C:199:ARG:HH22	1:C:201:GLN:HE21	1.43	0.66
1:D:184:VAL:HG13	1:D:284:PRO:HA	1.77	0.66
1:D:36:ALA:O	1:D:161:LEU:HD12	1.95	0.66
1:F:199:ARG:HH22	1:F:201:GLN:HE21	1.43	0.66
1:B:36:ALA:O	1:B:161:LEU:HD12	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:ALA:O	1:C:161:LEU:HD12	1.95	0.66
1:E:293:ARG:NH2	1:E:336:GLU:OE1	2.28	0.66
1:F:199:ARG:HH22	1:F:201:GLN:NE2	1.92	0.66
1:F:36:ALA:O	1:F:161:LEU:HD12	1.95	0.66
1:G:170:VAL:HB	1:G:178:ILE:HD11	1.76	0.66
1:A:199:ARG:HH22	1:A:201:GLN:NE2	1.92	0.66
1:F:295:GLN:O	1:F:296:LEU:HD23	1.95	0.66
1:F:61:ASN:CG	1:F:63:GLN:HG3	2.15	0.66
1:G:199:ARG:HH22	1:G:201:GLN:NE2	1.92	0.66
1:H:201:GLN:NE2	1:H:252:ASN:H	1.93	0.66
1:H:201:GLN:CG	1:H:280:THR:HG22	2.18	0.66
1:A:199:ARG:HH22	1:A:201:GLN:HE21	1.43	0.66
1:B:199:ARG:HH22	1:B:201:GLN:HE21	1.43	0.66
1:C:293:ARG:NH2	1:C:336:GLU:OE1	2.28	0.66
1:E:151:ARG:NH2	1:E:154:GLU:OE2	2.28	0.66
1:B:177:VAL:HG22	1:B:304:GLU:HB2	1.77	0.66
1:C:151:ARG:NH2	1:C:154:GLU:OE2	2.28	0.66
1:E:199:ARG:HH22	1:E:201:GLN:NE2	1.92	0.66
1:F:254:GLN:O	1:F:258:THR:HG23	1.94	0.66
1:F:61:ASN:HD21	1:F:63:GLN:CD	1.97	0.66
1:H:293:ARG:NH2	1:H:336:GLU:OE1	2.28	0.66
1:B:151:ARG:NH2	1:B:154:GLU:OE2	2.28	0.66
1:F:151:ARG:NH2	1:F:154:GLU:OE2	2.28	0.66
1:F:256:HIS:HD1	1:F:278:GLU:CD	1.97	0.66
1:A:216:THR:HG21	1:A:226:SER:HB3	1.76	0.66
1:D:201:GLN:NE2	1:D:252:ASN:H	1.93	0.66
1:D:215:ILE:HG22	1:D:217:HIS:CE1	2.31	0.66
1:G:151:ARG:NH2	1:G:154:GLU:OE2	2.28	0.66
1:A:293:ARG:NH2	1:A:336:GLU:OE1	2.28	0.66
1:A:295:GLN:O	1:A:296:LEU:HD23	1.95	0.66
1:D:151:ARG:NH2	1:D:154:GLU:OE2	2.28	0.66
1:D:216:THR:HG21	1:D:226:SER:HB3	1.76	0.66
1:D:293:ARG:NH2	1:D:336:GLU:OE1	2.28	0.66
1:E:36:ALA:O	1:E:161:LEU:HD12	1.95	0.66
1:D:295:GLN:O	1:D:296:LEU:HD23	1.95	0.66
1:H:256:HIS:HD1	1:H:278:GLU:CD	1.97	0.66
1:H:36:ALA:O	1:H:161:LEU:HD12	1.95	0.66
1:C:22:ARG:HD3	1:C:23:TYR:CE1	2.31	0.65
1:G:256:HIS:HD1	1:G:278:GLU:CD	1.97	0.65
1:G:295:GLN:O	1:G:296:LEU:HD23	1.95	0.65
1:B:295:GLN:O	1:B:296:LEU:HD23	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:ILE:HG22	1:C:254:GLN:N	2.11	0.65
1:G:223:ILE:CB	1:G:224:TYR:HD1	2.09	0.65
1:C:55:TYR:CE1	1:C:314:TYR:CD1	2.84	0.65
1:G:36:ALA:O	1:G:161:LEU:HD12	1.95	0.65
1:F:201:GLN:NE2	1:F:252:ASN:H	1.93	0.65
1:H:184:VAL:HG13	1:H:284:PRO:HA	1.77	0.65
1:D:61:ASN:OD1	1:D:61:ASN:N	2.30	0.65
1:G:201:GLN:NE2	1:G:252:ASN:H	1.93	0.65
1:C:254:GLN:O	1:C:258:THR:HG23	1.97	0.65
1:C:23:TYR:O	1:C:30:LEU:HD23	1.97	0.65
1:E:161:LEU:O	1:E:162:ARG:HG2	1.96	0.65
1:E:201:GLN:NE2	1:E:252:ASN:H	1.93	0.65
1:A:184:VAL:HG13	1:A:284:PRO:HA	1.77	0.65
1:C:184:VAL:HG13	1:C:284:PRO:HA	1.77	0.65
1:F:253:ILE:HG22	1:F:254:GLN:N	2.09	0.65
1:G:184:VAL:HG13	1:G:284:PRO:HA	1.77	0.65
1:C:23:TYR:HE2	1:C:330:PHE:HD2	1.43	0.65
1:D:201:GLN:CG	1:D:280:THR:HG22	2.18	0.65
1:B:171:ALA:HB1	1:B:303:THR:CG2	2.27	0.64
1:E:33:LYS:HE3	4:E:350:DTR:CZ2	2.27	0.64
1:G:223:ILE:CB	1:G:224:TYR:CD1	2.81	0.64
1:A:69:GLN:CB	1:A:110:MET:HE3	2.23	0.64
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.46	0.64
1:D:121:GLU:O	1:D:124:MET:HB2	1.98	0.64
1:A:253:ILE:HG12	1:F:42:PHE:CG	2.29	0.64
1:B:250:ILE:HD11	1:E:250:ILE:HD13	1.75	0.64
1:D:180:ASN:HD22	1:D:307:HIS:HD2	1.46	0.64
1:H:180:ASN:HD22	1:H:307:HIS:HD2	1.46	0.64
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.46	0.64
1:D:253:ILE:HG22	1:D:254:GLN:N	2.11	0.64
1:G:223:ILE:C	1:G:224:TYR:HD1	2.00	0.64
1:A:253:ILE:HA	1:F:42:PHE:CZ	2.33	0.64
1:C:180:ASN:HD22	1:C:307:HIS:HD2	1.46	0.64
1:E:180:ASN:HD22	1:E:307:HIS:HD2	1.46	0.64
1:G:223:ILE:HG22	1:G:224:TYR:CD1	2.33	0.64
1:E:22:ARG:CG	1:E:22:ARG:HH11	1.99	0.64
1:F:168:GLU:O	1:F:171:ALA:HB3	1.96	0.64
1:A:128:TYR:CD2	1:A:128:TYR:N	2.66	0.63
1:E:256:HIS:HD1	1:E:278:GLU:CD	1.97	0.63
1:A:256:HIS:HD1	1:A:278:GLU:CD	1.97	0.63
1:B:253:ILE:HG12	1:E:42:PHE:CG	2.33	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:180:ASN:HD22	1:G:307:HIS:HD2	1.46	0.63
1:B:192:ASP:OD1	1:B:194:LEU:HB2	1.99	0.63
1:E:2:ARG:HD3	4:E:350:DTR:CE2	2.28	0.63
1:D:192:ASP:OD1	1:D:194:LEU:HB2	1.99	0.62
1:H:224:TYR:HB2	1:H:242:PHE:CD2	2.32	0.62
1:C:256:HIS:HD1	1:C:278:GLU:CD	1.97	0.62
1:D:27:LEU:HD12	1:D:30:LEU:CB	2.09	0.62
1:E:192:ASP:OD1	1:E:194:LEU:HB2	1.99	0.62
1:D:82:PRO:HA	1:H:268:PRO:HB2	1.79	0.62
1:B:250:ILE:HD13	1:E:250:ILE:CD1	2.30	0.62
1:F:192:ASP:OD1	1:F:194:LEU:HB2	1.99	0.62
1:F:216:THR:HG21	1:F:226:SER:HB3	1.76	0.62
1:F:180:ASN:HD22	1:F:307:HIS:HD2	1.46	0.62
1:G:192:ASP:OD1	1:G:194:LEU:HB2	1.99	0.62
1:H:216:THR:HG21	1:H:226:SER:HB3	1.76	0.62
1:H:58:GLU:HG3	1:H:59:PRO:HD2	1.78	0.62
1:A:254:GLN:O	1:A:258:THR:HG23	2.00	0.62
1:G:223:ILE:CG2	1:G:224:TYR:CD1	2.83	0.62
1:E:138:ILE:HD11	1:E:231:PRO:O	2.00	0.62
1:F:138:ILE:HD11	1:F:231:PRO:O	2.00	0.62
1:D:223:ILE:HG12	1:D:224:TYR:HE1	1.61	0.62
1:F:58:GLU:HB3	1:F:59:PRO:CD	2.30	0.62
1:B:59:PRO:HG2	1:B:61:ASN:O	1.99	0.61
1:G:69:GLN:CB	1:G:110:MET:HE3	2.24	0.61
1:G:216:THR:HG21	1:G:226:SER:HB3	1.76	0.61
1:H:170:VAL:HB	1:H:178:ILE:HD11	1.82	0.61
1:C:192:ASP:OD1	1:C:194:LEU:HB2	1.99	0.61
1:A:20:HIS:CE1	1:A:155:ARG:HH11	2.19	0.61
1:A:192:ASP:OD1	1:A:194:LEU:HB2	1.99	0.61
1:H:192:ASP:OD1	1:H:194:LEU:HB2	1.99	0.61
1:B:20:HIS:CE1	1:B:155:ARG:HH11	2.19	0.61
1:D:252:ASN:OD1	1:D:254:GLN:HG2	2.01	0.61
1:D:171:ALA:C	1:D:173:GLY:H	2.02	0.61
1:D:252:ASN:CG	1:D:254:GLN:HG2	2.20	0.61
1:B:138:ILE:HD11	1:B:231:PRO:O	2.00	0.61
1:D:252:ASN:ND2	1:D:254:GLN:HG2	2.16	0.61
1:H:20:HIS:CE1	1:H:155:ARG:HH11	2.19	0.61
1:A:170:VAL:O	1:A:170:VAL:HG12	1.99	0.61
1:H:168:GLU:O	1:H:171:ALA:N	2.33	0.61
1:C:20:HIS:CE1	1:C:155:ARG:HH11	2.19	0.61
1:C:23:TYR:CE2	1:C:330:PHE:CD2	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:20:HIS:CE1	1:F:155:ARG:HH11	2.19	0.61
1:F:246:ASN:OD1	1:F:248:ASN:N	2.26	0.61
1:F:278:GLU:HG3	5:F:355:HOH:O	2.00	0.61
1:G:142:ARG:O	1:G:146:GLN:HG3	2.01	0.61
1:D:142:ARG:O	1:D:146:GLN:HG3	2.01	0.61
1:D:138:ILE:HD11	1:D:231:PRO:O	2.00	0.61
1:D:253:ILE:HG12	1:G:42:PHE:CE1	2.36	0.61
1:G:138:ILE:HD11	1:G:231:PRO:O	2.00	0.61
1:A:142:ARG:O	1:A:146:GLN:HG3	2.01	0.61
1:B:246:ASN:OD1	1:B:248:ASN:N	2.26	0.61
1:B:254:GLN:O	1:B:258:THR:HG23	2.00	0.61
1:B:59:PRO:CB	1:B:61:ASN:O	2.48	0.61
1:E:142:ARG:O	1:E:146:GLN:HG3	2.01	0.61
1:G:20:HIS:CE1	1:G:155:ARG:HH11	2.19	0.61
1:H:142:ARG:O	1:H:146:GLN:HG3	2.01	0.61
1:F:142:ARG:O	1:F:146:GLN:HG3	2.01	0.60
1:G:223:ILE:HG21	1:G:224:TYR:HE1	1.66	0.60
1:H:138:ILE:HD11	1:H:231:PRO:O	2.00	0.60
1:B:142:ARG:O	1:B:146:GLN:HG3	2.01	0.60
1:D:20:HIS:CE1	1:D:155:ARG:HH11	2.19	0.60
1:F:223:ILE:CG1	1:F:224:TYR:CD1	2.76	0.60
1:A:138:ILE:HD11	1:A:231:PRO:O	2.00	0.60
1:C:142:ARG:O	1:C:146:GLN:HG3	2.01	0.60
1:C:138:ILE:HD11	1:C:231:PRO:O	2.00	0.60
1:D:256:HIS:HD1	1:D:278:GLU:CD	1.97	0.60
1:E:58:GLU:CG	1:E:59:PRO:HD2	2.32	0.60
1:G:252:ASN:OD1	1:G:254:GLN:N	2.35	0.60
1:D:224:TYR:N	1:D:224:TYR:CD1	2.70	0.59
1:D:30:LEU:HD11	1:D:32:VAL:HG23	1.84	0.59
1:E:20:HIS:CE1	1:E:155:ARG:HH11	2.19	0.59
1:D:128:TYR:CD1	1:D:128:TYR:N	2.71	0.59
1:D:296:LEU:HD11	5:D:354:HOH:O	2.02	0.59
1:F:128:TYR:CD1	1:F:128:TYR:N	2.71	0.59
1:C:55:TYR:HD2	1:C:223:ILE:HD13	1.68	0.59
1:G:121:GLU:HA	1:G:124:MET:HE2	1.85	0.59
1:D:223:ILE:CG2	1:D:224:TYR:CD1	2.85	0.59
1:H:69:GLN:CB	1:H:110:MET:HE3	2.28	0.59
1:A:246:ASN:OD1	1:A:248:ASN:N	2.26	0.58
1:E:20:HIS:CE1	1:E:155:ARG:NH1	2.72	0.58
1:G:246:ASN:OD1	1:G:248:ASN:N	2.26	0.58
1:G:62:PRO:CG	1:G:63:GLN:HG3	2.31	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:HIS:CE1	1:B:155:ARG:NH1	2.72	0.58
1:E:168:GLU:O	1:E:171:ALA:HB3	2.04	0.58
1:G:20:HIS:CE1	1:G:155:ARG:NH1	2.71	0.58
1:B:225:ASN:ND2	1:B:240:GLY:O	2.35	0.58
1:C:20:HIS:CE1	1:C:155:ARG:NH1	2.72	0.58
1:G:253:ILE:HG22	1:G:254:GLN:N	2.16	0.58
1:H:20:HIS:CE1	1:H:155:ARG:NH1	2.72	0.58
1:D:269:THR:C	1:D:271:LYS:N	2.57	0.58
1:H:172:ARG:C	1:H:174:GLY:H	2.05	0.58
1:B:59:PRO:CG	1:B:61:ASN:O	2.51	0.58
1:F:195:LEU:HD12	1:F:285:VAL:O	2.04	0.58
1:A:20:HIS:CE1	1:A:155:ARG:NH1	2.71	0.58
1:C:136:SER:OG	1:C:137:LEU:N	2.37	0.58
1:C:195:LEU:HD12	1:C:285:VAL:O	2.04	0.58
1:D:195:LEU:HD12	1:D:285:VAL:O	2.04	0.58
1:F:92:VAL:CG2	1:F:138:ILE:HG13	2.34	0.58
1:H:92:VAL:CG2	1:H:138:ILE:HG13	2.34	0.58
1:B:253:ILE:HG12	1:E:42:PHE:CE1	2.38	0.58
1:G:195:LEU:HD12	1:G:285:VAL:O	2.04	0.58
1:B:83:ASN:O	1:B:86:ASN:N	2.37	0.57
1:D:20:HIS:CE1	1:D:155:ARG:NH1	2.71	0.57
1:D:92:VAL:CG2	1:D:138:ILE:HG13	2.34	0.57
1:B:253:ILE:CG1	1:E:42:PHE:CD1	2.84	0.57
1:G:83:ASN:O	1:G:86:ASN:N	2.37	0.57
1:A:83:ASN:O	1:A:86:ASN:N	2.37	0.57
1:B:136:SER:OG	1:B:137:LEU:N	2.37	0.57
1:H:136:SER:OG	1:H:137:LEU:N	2.37	0.57
1:D:83:ASN:O	1:D:86:ASN:N	2.37	0.57
1:F:69:GLN:CA	1:F:110:MET:HE2	2.35	0.57
1:C:92:VAL:CG2	1:C:138:ILE:HG13	2.34	0.57
1:H:170:VAL:HB	1:H:178:ILE:CD1	2.34	0.57
1:D:90:THR:CG2	5:D:369:HOH:O	2.46	0.57
1:G:136:SER:OG	1:G:137:LEU:N	2.37	0.57
1:D:252:ASN:OD1	1:D:254:GLN:N	2.37	0.57
1:H:122:LEU:C	1:H:124:MET:H	2.08	0.57
1:H:195:LEU:HD12	1:H:285:VAL:O	2.04	0.57
1:A:195:LEU:HD12	1:A:285:VAL:O	2.04	0.57
1:G:92:VAL:CG2	1:G:138:ILE:HG13	2.34	0.57
1:H:122:LEU:C	1:H:124:MET:N	2.57	0.57
1:B:92:VAL:CG2	1:B:138:ILE:HG13	2.34	0.57
1:C:83:ASN:O	1:C:86:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:SER:OG	1:F:137:LEU:N	2.37	0.57
1:F:20:HIS:CE1	1:F:155:ARG:NH1	2.71	0.57
1:D:136:SER:OG	1:D:137:LEU:N	2.37	0.57
1:D:223:ILE:HG13	1:D:224:TYR:HD1	1.57	0.57
1:D:223:ILE:C	1:D:224:TYR:CD1	2.76	0.57
1:C:128:TYR:N	1:C:128:TYR:CD2	2.73	0.57
1:C:89:LEU:HD23	1:C:138:ILE:O	2.05	0.56
1:E:92:VAL:CG2	1:E:138:ILE:HG13	2.34	0.56
1:H:83:ASN:O	1:H:86:ASN:N	2.37	0.56
1:A:136:SER:OG	1:A:137:LEU:N	2.37	0.56
1:A:92:VAL:CG2	1:A:138:ILE:HG13	2.34	0.56
1:D:139:LEU:HD21	1:D:144:TYR:CE2	2.41	0.56
1:D:246:ASN:OD1	1:D:248:ASN:N	2.26	0.56
1:E:83:ASN:O	1:E:86:ASN:N	2.37	0.56
1:F:139:LEU:HD21	1:F:144:TYR:CE2	2.41	0.56
1:F:83:ASN:O	1:F:86:ASN:N	2.37	0.56
1:H:89:LEU:HD23	1:H:138:ILE:O	2.05	0.56
1:B:105:PRO:HD3	1:B:132:TRP:CH2	2.41	0.56
1:B:195:LEU:HD12	1:B:285:VAL:O	2.04	0.56
1:D:89:LEU:HD23	1:D:138:ILE:O	2.05	0.56
1:H:139:LEU:HD21	1:H:144:TYR:CE2	2.41	0.56
1:A:121:GLU:O	1:A:124:MET:HG3	2.05	0.56
1:F:223:ILE:CG2	1:F:224:TYR:HD1	2.19	0.56
1:F:61:ASN:ND2	1:F:63:GLN:HG3	2.21	0.56
1:E:195:LEU:HD12	1:E:285:VAL:O	2.04	0.56
1:E:218:ASP:HB2	1:E:226:SER:HG	1.69	0.56
1:G:89:LEU:HD23	1:G:138:ILE:O	2.05	0.56
1:B:55:TYR:CE2	1:B:224:TYR:OH	2.58	0.56
1:E:139:LEU:HD21	1:E:144:TYR:CE2	2.41	0.56
1:A:139:LEU:HD21	1:A:144:TYR:CE2	2.41	0.56
1:C:139:LEU:HD21	1:C:144:TYR:CE2	2.41	0.56
1:A:89:LEU:HD23	1:A:138:ILE:O	2.06	0.56
1:C:105:PRO:HD3	1:C:132:TRP:CH2	2.41	0.56
1:D:170:VAL:CG1	1:D:178:ILE:HD13	2.36	0.56
1:F:89:LEU:HD23	1:F:138:ILE:O	2.06	0.56
1:H:105:PRO:HD3	1:H:132:TRP:CH2	2.41	0.55
1:E:89:LEU:HD23	1:E:138:ILE:O	2.06	0.55
1:B:89:LEU:HD23	1:B:138:ILE:O	2.05	0.55
1:C:252:ASN:OD1	1:C:254:GLN:N	2.40	0.55
1:E:160:PHE:CD1	1:E:162:ARG:NH2	2.75	0.55
1:A:250:ILE:CD1	1:F:250:ILE:CD1	2.80	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD13	1:F:250:ILE:HD13	1.87	0.55
1:A:253:ILE:HA	1:F:42:PHE:CE1	2.41	0.55
1:E:69:GLN:CB	1:E:110:MET:HE3	2.30	0.55
1:F:61:ASN:HD21	1:F:63:GLN:CG	2.19	0.55
1:G:139:LEU:HD21	1:G:144:TYR:CE2	2.41	0.55
1:F:105:PRO:HD3	1:F:132:TRP:CH2	2.41	0.55
1:F:97:LEU:HD11	1:F:125:PHE:CD2	2.42	0.55
1:H:23:TYR:CE2	1:H:330:PHE:HD2	2.25	0.55
1:H:254:GLN:O	1:H:258:THR:HG23	2.07	0.55
1:A:105:PRO:HD3	1:A:132:TRP:CH2	2.41	0.55
1:E:105:PRO:HD3	1:E:132:TRP:CH2	2.41	0.55
1:G:105:PRO:HD3	1:G:132:TRP:CH2	2.41	0.55
1:G:171:ALA:HA	1:G:175:ALA:CB	2.33	0.55
1:G:177:VAL:HG12	1:G:178:ILE:N	2.21	0.55
1:G:249:GLU:HB3	1:G:282:PHE:CZ	2.42	0.55
1:B:139:LEU:HD21	1:B:144:TYR:CE2	2.41	0.55
1:D:249:GLU:HB3	1:D:282:PHE:CZ	2.42	0.55
1:D:105:PRO:HD3	1:D:132:TRP:CH2	2.41	0.55
1:F:249:GLU:HB3	1:F:282:PHE:CZ	2.42	0.55
1:C:252:ASN:ND2	5:C:361:HOH:O	2.40	0.55
1:E:249:GLU:HB3	1:E:282:PHE:CZ	2.42	0.55
1:A:249:GLU:HB3	1:A:282:PHE:CZ	2.42	0.54
1:C:165:GLU:HA	1:C:165:GLU:OE1	2.07	0.54
1:C:246:ASN:OD1	1:C:248:ASN:N	2.26	0.54
1:G:2:ARG:N	1:G:176:ASP:OD2	2.31	0.54
1:H:58:GLU:HG2	1:H:59:PRO:HD2	1.87	0.54
1:G:23:TYR:CE2	1:G:330:PHE:HD2	2.25	0.54
1:B:167:PHE:O	1:B:171:ALA:N	2.40	0.54
1:C:249:GLU:HB3	1:C:282:PHE:CZ	2.42	0.54
1:D:254:GLN:O	1:D:258:THR:HG23	2.08	0.54
1:B:249:GLU:HB3	1:B:282:PHE:CZ	2.42	0.54
1:H:249:GLU:HB3	1:H:282:PHE:CZ	2.42	0.54
1:G:178:ILE:HG22	1:G:178:ILE:O	2.07	0.54
1:G:59:PRO:HG3	1:G:106:TYR:CE1	2.43	0.54
1:C:150:GLU:O	1:C:154:GLU:HG3	2.08	0.54
1:E:30:LEU:HD12	1:E:31:ASP:N	2.23	0.54
1:F:150:GLU:O	1:F:154:GLU:HG3	2.08	0.54
1:H:99:ARG:O	1:H:129:ARG:HG3	2.07	0.54
1:B:22:ARG:HD2	1:B:23:TYR:CE1	2.42	0.54
1:B:268:PRO:O	1:B:271:LYS:HB2	2.07	0.54
1:H:150:GLU:O	1:H:154:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:THR:C	1:C:271:LYS:H	2.11	0.54
1:F:1:MET:SD	1:F:177:VAL:HG23	2.48	0.54
1:B:69:GLN:CB	1:B:110:MET:HE2	2.28	0.54
1:B:168:GLU:O	1:B:171:ALA:N	2.41	0.54
1:D:21:GLU:HG3	1:D:155:ARG:NH2	2.23	0.53
1:D:27:LEU:HD12	1:D:30:LEU:CD2	2.39	0.53
1:G:69:GLN:CB	1:G:110:MET:CE	2.84	0.53
1:B:136:SER:O	1:B:137:LEU:HD23	2.09	0.53
1:E:21:GLU:HG3	1:E:155:ARG:NH2	2.23	0.53
1:A:150:GLU:O	1:A:154:GLU:HG3	2.08	0.53
1:B:150:GLU:O	1:B:154:GLU:HG3	2.08	0.53
1:C:136:SER:O	1:C:137:LEU:HD23	2.09	0.53
1:E:22:ARG:CG	1:E:22:ARG:NH1	2.66	0.53
1:F:136:SER:O	1:F:137:LEU:HD23	2.09	0.53
1:H:136:SER:O	1:H:137:LEU:HD23	2.09	0.53
1:D:136:SER:O	1:D:137:LEU:HD23	2.09	0.53
1:F:21:GLU:HG3	1:F:155:ARG:NH2	2.23	0.53
1:H:58:GLU:HG3	1:H:59:PRO:HD3	1.91	0.53
1:A:21:GLU:HG3	1:A:155:ARG:NH2	2.23	0.53
1:B:293:ARG:NH2	1:B:336:GLU:CD	2.61	0.53
1:C:21:GLU:HG3	1:C:155:ARG:NH2	2.23	0.53
1:H:246:ASN:OD1	1:H:248:ASN:N	2.26	0.53
1:A:23:TYR:CD2	1:A:334:LEU:HD12	2.43	0.53
1:E:150:GLU:O	1:E:154:GLU:HG3	2.08	0.53
1:F:69:GLN:HB2	1:F:110:MET:HE2	1.85	0.53
1:G:21:GLU:HG3	1:G:155:ARG:NH2	2.23	0.53
1:G:136:SER:O	1:G:137:LEU:HD23	2.09	0.53
1:G:150:GLU:O	1:G:154:GLU:HG3	2.08	0.53
1:H:21:GLU:HG3	1:H:155:ARG:NH2	2.23	0.53
1:A:89:LEU:HA	1:A:138:ILE:O	2.09	0.53
1:D:171:ALA:C	1:D:173:GLY:N	2.61	0.53
1:E:293:ARG:NE	1:E:333:VAL:HG23	2.24	0.53
1:H:215:ILE:HG22	1:H:217:HIS:CE1	2.43	0.53
1:H:293:ARG:NE	1:H:333:VAL:HG23	2.24	0.53
1:C:89:LEU:HA	1:C:138:ILE:O	2.09	0.53
1:C:293:ARG:NE	1:C:333:VAL:HG23	2.24	0.52
1:D:150:GLU:O	1:D:154:GLU:HG3	2.08	0.52
1:D:223:ILE:CG2	1:D:224:TYR:HD1	2.20	0.52
1:E:136:SER:O	1:E:137:LEU:HD23	2.09	0.52
1:E:58:GLU:CB	1:E:59:PRO:HD2	2.38	0.52
1:G:89:LEU:HA	1:G:138:ILE:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLU:HG3	1:B:155:ARG:NH2	2.23	0.52
1:C:96:ASN:OD1	1:C:217:HIS:HE1	1.92	0.52
1:C:22:ARG:HG2	1:C:23:TYR:CE1	2.45	0.52
1:D:89:LEU:HA	1:D:138:ILE:O	2.09	0.52
1:A:293:ARG:NE	1:A:333:VAL:HG23	2.24	0.52
1:D:27:LEU:HD12	1:D:30:LEU:HD22	1.90	0.52
1:G:293:ARG:NE	1:G:333:VAL:HG23	2.24	0.52
1:C:253:ILE:CG1	1:H:42:PHE:CD1	2.88	0.52
1:A:136:SER:O	1:A:137:LEU:HD23	2.09	0.52
1:A:252:ASN:OD1	1:A:254:GLN:HG2	2.10	0.52
1:D:293:ARG:NE	1:D:333:VAL:HG23	2.24	0.52
1:B:293:ARG:NE	1:B:333:VAL:HG23	2.24	0.52
1:E:2:ARG:HD3	4:E:350:DTR:CG	2.40	0.52
1:G:210:LEU:HB3	5:G:352:HOH:O	2.10	0.52
1:E:136:SER:OG	1:E:137:LEU:N	2.37	0.52
1:F:89:LEU:HA	1:F:138:ILE:O	2.09	0.52
1:B:251:ASN:HA	1:B:280:THR:HG21	1.92	0.52
1:H:89:LEU:HA	1:H:138:ILE:O	2.09	0.52
1:F:293:ARG:NE	1:F:333:VAL:HG23	2.24	0.52
1:B:89:LEU:HA	1:B:138:ILE:O	2.09	0.52
1:E:89:LEU:HA	1:E:138:ILE:O	2.09	0.52
1:F:223:ILE:CG2	1:F:224:TYR:CD1	2.91	0.52
1:G:251:ASN:HA	1:G:280:THR:HG21	1.92	0.51
1:D:69:GLN:CB	1:D:110:MET:HE3	2.32	0.51
1:G:122:LEU:O	1:G:125:PHE:O	2.28	0.51
1:G:23:TYR:CD2	1:G:330:PHE:CD2	2.98	0.51
1:G:293:ARG:NH2	1:G:336:GLU:CD	2.61	0.51
1:A:287:PRO:HB2	1:A:288:GLN:CD	2.31	0.51
1:B:119:PRO:HD3	5:B:356:HOH:O	2.11	0.51
1:C:251:ASN:HA	1:C:280:THR:HG21	1.92	0.51
1:D:224:TYR:HB2	1:D:242:PHE:HB2	1.91	0.51
1:D:268:PRO:HB2	1:H:82:PRO:HA	1.92	0.51
1:F:1:MET:SD	1:F:177:VAL:CG2	2.99	0.51
1:F:223:ILE:CG1	1:F:224:TYR:HD1	2.17	0.51
1:F:22:ARG:HG3	1:F:22:ARG:O	2.11	0.51
1:E:252:ASN:OD1	1:E:252:ASN:C	2.49	0.51
1:F:251:ASN:HA	1:F:280:THR:HG21	1.92	0.51
1:F:252:ASN:C	1:F:252:ASN:OD1	2.49	0.51
1:G:252:ASN:C	1:G:252:ASN:OD1	2.49	0.51
1:G:59:PRO:HG3	1:G:106:TYR:CE2	2.44	0.51
1:D:252:ASN:C	1:D:252:ASN:OD1	2.49	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:252:ASN:OD1	1:H:252:ASN:C	2.49	0.51
1:H:251:ASN:HA	1:H:280:THR:HG21	1.92	0.51
1:C:293:ARG:NH2	1:C:336:GLU:CD	2.62	0.51
1:A:251:ASN:HA	1:A:280:THR:HG21	1.92	0.51
1:A:55:TYR:HB2	1:A:314:TYR:OH	2.11	0.51
1:C:252:ASN:C	1:C:252:ASN:OD1	2.49	0.51
1:C:23:TYR:CD2	1:C:330:PHE:CD2	2.99	0.51
1:D:251:ASN:HA	1:D:280:THR:HG21	1.92	0.51
1:D:249:GLU:HG3	1:G:250:ILE:HD12	1.92	0.51
1:B:121:GLU:HA	1:B:124:MET:HE2	1.93	0.51
1:B:311:HIS:O	1:B:314:TYR:CD1	2.64	0.51
1:D:61:ASN:ND2	1:D:63:GLN:HE21	1.95	0.51
1:A:11:ILE:HD12	1:A:311:HIS:CE1	2.47	0.50
1:A:171:ALA:HB1	1:A:303:THR:HG21	1.93	0.50
1:D:27:LEU:CD1	1:D:30:LEU:HD22	2.41	0.50
1:B:250:ILE:HD11	1:E:250:ILE:HD11	1.92	0.50
1:F:69:GLN:N	1:F:110:MET:HE2	2.26	0.50
1:B:252:ASN:OD1	1:B:252:ASN:C	2.49	0.50
1:B:293:ARG:HE	1:B:333:VAL:CG2	2.25	0.50
1:E:69:GLN:N	1:E:110:MET:HE2	2.26	0.50
4:F:350:DTR:HE3	4:F:350:DTR:H	1.75	0.50
1:A:252:ASN:C	1:A:252:ASN:OD1	2.49	0.50
1:F:69:GLN:CB	1:F:110:MET:CE	2.84	0.50
1:G:144:TYR:CE2	1:G:319:HIS:NE2	2.80	0.50
1:D:11:ILE:HD12	1:D:311:HIS:CE1	2.47	0.50
1:E:246:ASN:OD1	1:E:248:ASN:N	2.26	0.50
1:F:11:ILE:HD12	1:F:311:HIS:CE1	2.47	0.50
1:G:11:ILE:HD12	1:G:311:HIS:CE1	2.47	0.50
1:H:58:GLU:CG	1:H:59:PRO:CD	2.83	0.50
1:A:144:TYR:CE2	1:A:319:HIS:NE2	2.80	0.50
1:C:22:ARG:HD3	1:C:23:TYR:CZ	2.47	0.50
1:D:69:GLN:CB	1:D:110:MET:CE	2.83	0.50
1:D:265:ARG:HH11	1:D:265:ARG:HG3	1.76	0.50
1:G:165:GLU:OE1	1:G:165:GLU:HA	2.12	0.50
1:G:293:ARG:HE	1:G:333:VAL:CG2	2.25	0.50
1:H:144:TYR:CE2	1:H:319:HIS:NE2	2.80	0.50
1:B:69:GLN:N	1:B:110:MET:HE1	2.26	0.50
1:B:144:TYR:CE2	1:B:319:HIS:NE2	2.80	0.50
1:C:293:ARG:HE	1:C:333:VAL:CG2	2.25	0.50
1:D:69:GLN:CA	1:D:110:MET:HE2	2.42	0.50
1:D:265:ARG:NH1	1:D:265:ARG:HG3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:GLN:N	1:D:110:MET:HE2	2.26	0.50
1:E:144:TYR:CE2	1:E:319:HIS:NE2	2.80	0.50
1:F:17:LEU:CA	1:F:152:LEU:HD21	2.42	0.50
1:A:17:LEU:CA	1:A:152:LEU:HD21	2.42	0.50
1:B:128:TYR:N	1:B:128:TYR:HD1	2.07	0.50
1:D:144:TYR:CE2	1:D:319:HIS:NE2	2.80	0.50
1:E:251:ASN:HA	1:E:280:THR:HG21	1.92	0.50
1:E:59:PRO:HB2	1:E:61:ASN:O	2.12	0.50
1:G:223:ILE:C	1:G:224:TYR:CD1	2.83	0.50
1:H:11:ILE:HD12	1:H:311:HIS:CE1	2.47	0.50
1:B:11:ILE:HD12	1:B:311:HIS:CE1	2.47	0.50
1:F:144:TYR:CE2	1:F:319:HIS:NE2	2.80	0.50
1:A:293:ARG:HE	1:A:333:VAL:CG2	2.25	0.49
1:F:252:ASN:OD1	1:F:254:GLN:N	2.45	0.49
1:G:17:LEU:CA	1:G:152:LEU:HD21	2.42	0.49
1:H:69:GLN:N	1:H:110:MET:HE2	2.26	0.49
1:A:22:ARG:HG2	1:A:23:TYR:CE1	2.47	0.49
1:B:170:VAL:HG12	1:B:175:ALA:CB	2.42	0.49
1:B:250:ILE:CD1	1:E:250:ILE:HD11	2.40	0.49
1:C:112:LEU:HB2	1:C:135:THR:HB	1.95	0.49
1:F:293:ARG:HE	1:F:333:VAL:CG2	2.25	0.49
1:H:293:ARG:NH2	1:H:336:GLU:CD	2.61	0.49
1:C:268:PRO:HB2	1:G:82:PRO:HA	1.94	0.49
1:C:269:THR:C	1:C:271:LYS:N	2.63	0.49
1:A:97:LEU:HB3	1:A:128:TYR:CG	2.47	0.49
1:A:251:ASN:OD1	1:A:280:THR:CG2	2.59	0.49
1:C:17:LEU:CA	1:C:152:LEU:HD21	2.42	0.49
1:D:293:ARG:HE	1:D:333:VAL:CG2	2.24	0.49
1:F:130:TYR:CD1	1:F:131:GLY:N	2.81	0.49
1:G:22:ARG:O	1:G:22:ARG:CG	2.60	0.49
1:H:162:ARG:O	2:H:348:FAD:H2A	2.12	0.49
1:A:69:GLN:N	1:A:110:MET:HE2	2.27	0.49
1:C:130:TYR:CD1	1:C:131:GLY:N	2.81	0.49
1:G:166:SER:O	1:G:170:VAL:HG23	2.12	0.49
1:H:112:LEU:HB2	1:H:135:THR:HB	1.95	0.49
1:A:130:TYR:CD1	1:A:131:GLY:N	2.81	0.49
1:B:17:LEU:CA	1:B:152:LEU:HD21	2.42	0.49
1:C:144:TYR:CE2	1:C:319:HIS:NE2	2.80	0.49
1:D:170:VAL:HG12	1:D:178:ILE:CD1	2.42	0.49
1:D:17:LEU:CA	1:D:152:LEU:HD21	2.42	0.49
1:D:199:ARG:NH2	1:D:201:GLN:HE21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ARG:HH21	1:E:154:GLU:CD	2.16	0.49
1:C:11:ILE:HD12	1:C:311:HIS:CE1	2.47	0.49
1:E:11:ILE:HD12	1:E:311:HIS:CE1	2.47	0.49
1:G:130:TYR:CD1	1:G:131:GLY:N	2.81	0.49
1:G:170:VAL:HB	1:G:178:ILE:CD1	2.42	0.49
1:H:17:LEU:CA	1:H:152:LEU:HD21	2.42	0.49
1:C:166:SER:O	1:C:169:GLU:HB3	2.13	0.49
1:A:324:LEU:O	1:A:327:ALA:HB3	2.13	0.49
1:D:223:ILE:CB	1:D:224:TYR:HD1	2.26	0.49
1:D:251:ASN:OD1	1:D:280:THR:CG2	2.59	0.49
1:E:293:ARG:HE	1:E:333:VAL:CG2	2.24	0.49
1:G:151:ARG:HH21	1:G:154:GLU:CD	2.16	0.49
1:A:165:GLU:HB3	1:A:169:GLU:CD	2.34	0.49
1:C:22:ARG:CD	1:C:23:TYR:CE1	2.96	0.49
1:C:24:HIS:HD2	1:C:30:LEU:H	1.60	0.49
1:D:151:ARG:HH21	1:D:154:GLU:CD	2.16	0.49
1:D:55:TYR:N	1:D:55:TYR:CD1	2.77	0.49
1:E:166:SER:O	1:E:169:GLU:HB3	2.13	0.49
1:G:166:SER:O	1:G:169:GLU:HB3	2.13	0.49
1:H:293:ARG:HE	1:H:333:VAL:CG2	2.24	0.49
1:B:55:TYR:CE1	1:B:314:TYR:CD1	2.97	0.48
1:D:112:LEU:HB2	1:D:135:THR:HB	1.94	0.48
1:D:130:TYR:CD1	1:D:131:GLY:N	2.81	0.48
1:E:130:TYR:CD1	1:E:131:GLY:N	2.81	0.48
1:E:17:LEU:CA	1:E:152:LEU:HD21	2.42	0.48
1:E:256:HIS:CE1	1:E:278:GLU:OE2	2.64	0.48
1:F:11:ILE:HG13	2:F:348:FAD:O2P	2.13	0.48
1:A:151:ARG:HH21	1:A:154:GLU:CD	2.16	0.48
1:B:256:HIS:CE1	1:B:278:GLU:OE2	2.64	0.48
1:D:166:SER:O	1:D:169:GLU:HB3	2.13	0.48
1:D:242:PHE:C	1:D:242:PHE:CD1	2.87	0.48
1:D:324:LEU:O	1:D:327:ALA:HB3	2.13	0.48
1:E:173:GLY:O	4:E:350:DTR:HB3	2.13	0.48
1:G:69:GLN:N	1:G:110:MET:HE2	2.27	0.48
1:A:166:SER:O	1:A:169:GLU:HB3	2.13	0.48
1:B:130:TYR:CD1	1:B:131:GLY:N	2.81	0.48
1:B:324:LEU:O	1:B:327:ALA:HB3	2.13	0.48
1:D:249:GLU:HG3	1:G:250:ILE:CD1	2.44	0.48
1:G:324:LEU:O	1:G:327:ALA:HB3	2.13	0.48
1:H:166:SER:O	1:H:169:GLU:HB3	2.13	0.48
1:B:268:PRO:HB2	1:F:82:PRO:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:TYR:HD1	1:D:55:TYR:N	2.12	0.48
1:F:151:ARG:HH21	1:F:154:GLU:CD	2.16	0.48
1:F:242:PHE:CD1	1:F:242:PHE:C	2.87	0.48
1:F:61:ASN:ND2	1:F:63:GLN:CG	2.77	0.48
1:H:252:ASN:OD1	1:H:254:GLN:N	2.46	0.48
1:B:11:ILE:HG13	2:B:348:FAD:O2P	2.13	0.48
1:B:199:ARG:NH2	1:B:201:GLN:HE21	2.10	0.48
1:E:112:LEU:HB2	1:E:135:THR:HB	1.95	0.48
1:F:161:LEU:O	1:F:162:ARG:HD2	2.12	0.48
1:F:166:SER:O	1:F:169:GLU:HB3	2.13	0.48
1:H:130:TYR:CD1	1:H:131:GLY:N	2.81	0.48
1:H:324:LEU:O	1:H:327:ALA:HB3	2.13	0.48
1:B:69:GLN:CB	1:B:110:MET:CE	2.84	0.48
1:E:251:ASN:OD1	1:E:280:THR:CG2	2.59	0.48
1:E:256:HIS:CD2	1:E:256:HIS:C	2.87	0.48
1:G:23:TYR:CD2	1:G:330:PHE:HD2	2.32	0.48
1:A:242:PHE:CD1	1:A:242:PHE:C	2.87	0.48
1:C:151:ARG:HH21	1:C:154:GLU:CD	2.16	0.48
1:D:332:LYS:O	1:D:336:GLU:HG3	2.14	0.48
1:E:11:ILE:HG13	2:E:348:FAD:O2P	2.14	0.48
1:F:324:LEU:O	1:F:327:ALA:HB3	2.13	0.48
1:G:269:THR:C	1:G:271:LYS:N	2.66	0.48
1:A:11:ILE:HG13	2:A:348:FAD:O2P	2.13	0.48
1:B:256:HIS:C	1:B:256:HIS:CD2	2.87	0.48
1:D:11:ILE:HG13	2:D:348:FAD:O2P	2.14	0.48
1:E:69:GLN:CB	1:E:110:MET:CE	2.84	0.48
1:E:242:PHE:CD1	1:E:242:PHE:C	2.87	0.48
1:F:112:LEU:HB2	1:F:135:THR:HB	1.95	0.48
1:A:332:LYS:O	1:A:336:GLU:HG3	2.14	0.48
1:B:151:ARG:HH21	1:B:154:GLU:CD	2.16	0.48
1:E:332:LYS:O	1:E:336:GLU:HG3	2.14	0.48
1:G:11:ILE:HG13	2:G:348:FAD:O2P	2.14	0.48
1:G:332:LYS:O	1:G:336:GLU:HG3	2.14	0.48
1:A:313:GLY:C	1:A:314:TYR:CD1	2.87	0.48
1:B:166:SER:O	1:B:169:GLU:HB3	2.13	0.48
1:B:22:ARG:CD	1:B:22:ARG:O	2.61	0.48
1:B:278:GLU:C	1:B:279:TYR:CD1	2.88	0.48
1:B:55:TYR:CD1	1:B:55:TYR:N	2.82	0.48
1:D:256:HIS:C	1:D:256:HIS:CD2	2.87	0.48
1:G:168:GLU:O	1:G:171:ALA:HB3	2.13	0.48
1:G:278:GLU:C	1:G:279:TYR:CD1	2.88	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PRO:HB2	1:A:107:TRP:CE2	2.49	0.47
1:B:105:PRO:HB2	1:B:107:TRP:CE2	2.49	0.47
1:C:230:ILE:HA	1:C:231:PRO:HD2	1.75	0.47
1:C:242:PHE:CD1	1:C:242:PHE:C	2.87	0.47
1:C:278:GLU:C	1:C:279:TYR:CD1	2.88	0.47
1:C:332:LYS:O	1:C:336:GLU:HG3	2.14	0.47
1:C:51:LEU:HD12	1:C:52:TRP:N	2.29	0.47
1:D:105:PRO:HB2	1:D:107:TRP:CE2	2.49	0.47
1:D:170:VAL:HG11	1:D:178:ILE:HD13	1.96	0.47
1:E:105:PRO:HB2	1:E:107:TRP:CE2	2.49	0.47
1:F:251:ASN:OD1	1:F:280:THR:CG2	2.59	0.47
1:F:278:GLU:C	1:F:279:TYR:CD1	2.88	0.47
1:G:105:PRO:HB2	1:G:107:TRP:CE2	2.49	0.47
1:G:223:ILE:HG22	1:G:224:TYR:CE1	2.49	0.47
1:G:256:HIS:CD2	1:G:256:HIS:C	2.87	0.47
1:A:278:GLU:C	1:A:279:TYR:CD1	2.88	0.47
1:B:332:LYS:O	1:B:336:GLU:HG3	2.14	0.47
1:C:256:HIS:CD2	1:C:256:HIS:C	2.87	0.47
1:G:242:PHE:CD1	1:G:242:PHE:C	2.87	0.47
1:H:251:ASN:OD1	1:H:280:THR:CG2	2.59	0.47
1:H:35:TYR:CZ	1:H:162:ARG:NH1	2.83	0.47
1:A:112:LEU:HB2	1:A:135:THR:HB	1.95	0.47
1:B:112:LEU:HB2	1:B:135:THR:HB	1.95	0.47
1:E:252:ASN:OD1	1:E:254:GLN:N	2.47	0.47
1:E:324:LEU:O	1:E:327:ALA:HB3	2.13	0.47
1:E:58:GLU:CB	1:E:59:PRO:CD	2.92	0.47
1:F:69:GLN:CB	1:F:110:MET:HE2	2.43	0.47
1:D:195:LEU:HA	1:D:285:VAL:O	2.14	0.47
1:E:88:GLY:HA2	1:E:233:LEU:HD11	1.97	0.47
1:F:3:VAL:HB	1:F:32:VAL:HG22	1.97	0.47
1:F:293:ARG:NH2	1:F:336:GLU:CD	2.61	0.47
1:H:256:HIS:CD2	1:H:256:HIS:C	2.87	0.47
1:H:195:LEU:HA	1:H:285:VAL:O	2.14	0.47
1:A:3:VAL:HB	1:A:32:VAL:HG22	1.97	0.47
1:A:51:LEU:HD12	1:A:52:TRP:N	2.29	0.47
1:B:242:PHE:C	1:B:242:PHE:CD1	2.87	0.47
1:B:88:GLY:HA2	1:B:233:LEU:HD11	1.97	0.47
1:D:278:GLU:C	1:D:279:TYR:CD1	2.88	0.47
1:E:128:TYR:CD1	1:E:128:TYR:N	2.82	0.47
1:E:51:LEU:HD12	1:E:52:TRP:N	2.29	0.47
1:G:112:LEU:HB2	1:G:135:THR:HB	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:195:LEU:HA	1:G:285:VAL:O	2.14	0.47
1:D:253:ILE:CG1	1:G:42:PHE:CD1	2.84	0.47
1:A:256:HIS:C	1:A:256:HIS:CD2	2.87	0.47
1:C:105:PRO:HB2	1:C:107:TRP:CE2	2.49	0.47
1:C:69:GLN:N	1:C:110:MET:HE2	2.29	0.47
1:D:3:VAL:HB	1:D:32:VAL:HG22	1.97	0.47
1:D:88:GLY:HA2	1:D:233:LEU:HD11	1.97	0.47
1:G:22:ARG:O	1:G:22:ARG:HG2	2.13	0.47
1:H:224:TYR:HB2	1:H:242:PHE:HB2	1.96	0.47
1:H:332:LYS:O	1:H:336:GLU:HG3	2.14	0.47
1:H:11:ILE:HG13	2:H:348:FAD:O2P	2.14	0.47
1:A:208:PRO:HB2	1:E:233:LEU:O	2.15	0.47
1:A:88:GLY:HA2	1:A:233:LEU:HD11	1.97	0.47
1:A:242:PHE:HD1	1:A:242:PHE:C	2.18	0.47
1:B:201:GLN:HA	1:B:279:TYR:O	2.15	0.47
1:C:195:LEU:HA	1:C:285:VAL:O	2.14	0.47
1:C:11:ILE:HG13	2:C:348:FAD:O2P	2.13	0.47
1:E:278:GLU:C	1:E:279:TYR:CD1	2.88	0.47
1:F:51:LEU:HD12	1:F:52:TRP:N	2.29	0.47
1:G:30:LEU:C	1:G:30:LEU:HD12	2.32	0.47
1:H:105:PRO:HB2	1:H:107:TRP:CE2	2.49	0.47
1:A:195:LEU:HA	1:A:285:VAL:O	2.14	0.47
1:C:3:VAL:HB	1:C:32:VAL:HG22	1.97	0.47
1:D:144:TYR:HE2	1:D:319:HIS:NE2	2.13	0.47
1:D:51:LEU:HD12	1:D:52:TRP:N	2.29	0.47
1:G:144:TYR:HE2	1:G:319:HIS:NE2	2.13	0.47
1:H:201:GLN:HA	1:H:279:TYR:O	2.15	0.47
1:A:144:TYR:HE2	1:A:319:HIS:NE2	2.13	0.47
1:B:139:LEU:HD21	1:B:144:TYR:CD2	2.50	0.47
1:B:51:LEU:HD12	1:B:52:TRP:N	2.29	0.47
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.71	0.47
1:C:324:LEU:O	1:C:327:ALA:HB3	2.13	0.47
1:E:293:ARG:NH2	1:E:336:GLU:CD	2.61	0.47
1:F:256:HIS:CD2	1:F:256:HIS:C	2.87	0.47
1:G:51:LEU:HD12	1:G:52:TRP:N	2.29	0.47
1:H:129:ARG:O	1:H:130:TYR:HB2	2.14	0.47
1:H:151:ARG:HH21	1:H:154:GLU:CD	2.16	0.47
1:H:242:PHE:CD1	1:H:242:PHE:C	2.87	0.47
1:H:144:TYR:HE2	1:H:319:HIS:NE2	2.13	0.47
1:H:51:LEU:HD12	1:H:52:TRP:N	2.29	0.47
1:B:127:ASP:HB2	1:B:128:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ARG:NE	1:C:333:VAL:CG2	2.78	0.47
1:D:293:ARG:NE	1:D:333:VAL:CG2	2.78	0.47
1:D:69:GLN:HB2	1:D:110:MET:HE2	1.93	0.47
1:E:69:GLN:CA	1:E:110:MET:HE2	2.44	0.47
1:E:195:LEU:HA	1:E:285:VAL:O	2.14	0.47
1:H:242:PHE:HD1	1:H:242:PHE:C	2.18	0.47
1:E:144:TYR:HE2	1:E:319:HIS:NE2	2.13	0.47
1:F:88:GLY:HA2	1:F:233:LEU:HD11	1.97	0.47
1:F:195:LEU:HA	1:F:285:VAL:O	2.14	0.47
1:G:216:THR:CG2	1:G:217:HIS:N	2.75	0.47
1:G:3:VAL:HB	1:G:32:VAL:HG22	1.97	0.47
1:H:278:GLU:C	1:H:279:TYR:CD1	2.88	0.47
1:H:293:ARG:NE	1:H:333:VAL:CG2	2.78	0.47
1:A:293:ARG:NE	1:A:333:VAL:CG2	2.78	0.46
1:B:160:PHE:C	1:B:162:ARG:HG3	2.36	0.46
1:B:242:PHE:C	1:B:242:PHE:HD1	2.18	0.46
1:C:69:GLN:CB	1:C:110:MET:CE	2.84	0.46
1:D:60:SER:HB2	1:D:61:ASN:OD1	2.15	0.46
1:E:122:LEU:HD23	1:E:122:LEU:HA	1.70	0.46
1:B:256:HIS:HB2	1:E:42:PHE:HZ	1.80	0.46
1:F:105:PRO:HB2	1:F:107:TRP:CE2	2.49	0.46
1:G:250:ILE:HD12	1:G:250:ILE:HG23	1.44	0.46
1:H:61:ASN:O	1:H:64:GLU:HB2	2.15	0.46
1:H:88:GLY:HA2	1:H:233:LEU:HD11	1.97	0.46
1:C:195:LEU:HA	1:C:195:LEU:HD12	1.63	0.46
1:D:128:TYR:H	1:D:128:TYR:HD1	1.63	0.46
1:E:1:MET:HB2	1:E:176:ASP:OD2	2.15	0.46
1:E:201:GLN:HA	1:E:279:TYR:O	2.15	0.46
1:F:139:LEU:HD21	1:F:144:TYR:CD2	2.50	0.46
1:F:144:TYR:HE2	1:F:319:HIS:NE2	2.13	0.46
1:F:256:HIS:CE1	1:F:278:GLU:OE2	2.64	0.46
1:G:30:LEU:HD12	1:G:31:ASP:H	1.74	0.46
1:G:88:GLY:HA2	1:G:233:LEU:HD11	1.97	0.46
1:B:22:ARG:HD2	1:B:22:ARG:O	2.14	0.46
1:B:251:ASN:OD1	1:B:280:THR:CG2	2.59	0.46
1:C:201:GLN:HA	1:C:279:TYR:O	2.15	0.46
1:D:139:LEU:HD21	1:D:144:TYR:CD2	2.50	0.46
1:E:242:PHE:HD1	1:E:242:PHE:C	2.18	0.46
1:F:332:LYS:O	1:F:336:GLU:HG3	2.14	0.46
1:G:199:ARG:NH2	1:G:201:GLN:HE21	2.10	0.46
1:H:139:LEU:HD21	1:H:144:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:199:ARG:NH2	1:H:201:GLN:HE21	2.10	0.46
1:H:3:VAL:HB	1:H:32:VAL:HG22	1.97	0.46
1:A:69:GLN:CB	1:A:110:MET:CE	2.83	0.46
1:C:242:PHE:HD1	1:C:242:PHE:C	2.18	0.46
1:D:122:LEU:HD23	1:D:122:LEU:HA	1.70	0.46
1:E:139:LEU:HD21	1:E:144:TYR:CD2	2.50	0.46
1:E:199:ARG:NH2	1:E:201:GLN:HE21	2.10	0.46
1:E:293:ARG:NE	1:E:333:VAL:CG2	2.78	0.46
1:D:253:ILE:HA	1:G:42:PHE:CE1	2.51	0.46
1:H:76:LEU:HA	1:H:76:LEU:HD23	1.62	0.46
1:B:117:LEU:HD21	1:B:133:PHE:HB2	1.98	0.46
1:E:117:LEU:HD21	1:E:133:PHE:HB2	1.98	0.46
1:F:293:ARG:NE	1:F:333:VAL:CG2	2.78	0.46
1:H:13:LEU:HA	1:H:13:LEU:HD23	1.61	0.46
1:H:208:PRO:HD2	1:H:209:TRP:CE3	2.51	0.46
1:A:117:LEU:HD21	1:A:133:PHE:HB2	1.98	0.46
1:F:201:GLN:HA	1:F:279:TYR:O	2.15	0.46
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.56	0.46
1:G:201:GLN:HA	1:G:279:TYR:O	2.15	0.46
1:A:139:LEU:HD21	1:A:144:TYR:CD2	2.50	0.46
1:A:201:GLN:HA	1:A:279:TYR:O	2.15	0.46
1:A:162:ARG:O	2:A:348:FAD:H2A	2.16	0.46
1:B:195:LEU:HA	1:B:285:VAL:O	2.14	0.46
1:B:3:VAL:HB	1:B:32:VAL:HG22	1.97	0.46
1:C:139:LEU:HD21	1:C:144:TYR:CD2	2.50	0.46
1:C:208:PRO:HD2	1:C:209:TRP:CE3	2.51	0.46
1:F:230:ILE:HA	1:F:231:PRO:HD2	1.75	0.46
1:H:224:TYR:CB	1:H:242:PHE:HD2	2.23	0.46
1:B:208:PRO:HD2	1:B:209:TRP:CE3	2.51	0.46
1:B:144:TYR:HE2	1:B:319:HIS:NE2	2.13	0.46
1:D:201:GLN:HA	1:D:279:TYR:O	2.15	0.46
1:D:269:THR:O	1:D:271:LYS:N	2.49	0.46
1:E:201:GLN:HG3	1:E:280:THR:CG2	2.24	0.46
1:F:224:TYR:HE2	3:F:349:ITR:O	1.99	0.46
1:F:270:LEU:HD23	1:F:270:LEU:HA	1.71	0.46
1:G:269:THR:C	1:G:271:LYS:H	2.17	0.46
1:H:128:TYR:N	1:H:128:TYR:CD1	2.84	0.46
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.56	0.46
1:H:69:GLN:CA	1:H:110:MET:HE2	2.46	0.46
1:B:121:GLU:O	1:B:124:MET:HB2	2.16	0.46
1:C:97:LEU:HB3	1:C:128:TYR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:ARG:HB3	4:E:350:DTR:CH2	2.45	0.46
1:F:208:PRO:HD2	1:F:209:TRP:CE3	2.51	0.46
1:G:117:LEU:HD21	1:G:133:PHE:HB2	1.98	0.46
1:G:1:MET:O	1:G:30:LEU:HD13	2.15	0.46
1:H:69:GLN:CB	1:H:110:MET:CE	2.84	0.46
1:H:168:GLU:CA	1:H:171:ALA:HB3	2.40	0.46
1:A:195:LEU:HA	1:A:195:LEU:HD12	1.63	0.46
1:A:90:THR:HG21	1:E:209:TRP:HD1	1.81	0.46
1:B:76:LEU:HD23	1:B:76:LEU:HA	1.62	0.46
1:E:208:PRO:HD2	1:E:209:TRP:CE3	2.51	0.46
1:A:76:LEU:HA	1:A:76:LEU:HD23	1.62	0.45
1:B:120:ARG:HH22	1:F:110:MET:C	2.19	0.45
1:C:236:VAL:HG12	1:C:237:THR:N	2.31	0.45
1:C:43:THR:OG1	1:C:45:THR:HB	2.16	0.45
1:C:88:GLY:HA2	1:C:233:LEU:HD11	1.97	0.45
1:E:3:VAL:HB	1:E:32:VAL:HG22	1.97	0.45
1:G:139:LEU:HD21	1:G:144:TYR:CD2	2.50	0.45
1:D:250:ILE:CD1	1:G:249:GLU:HG3	2.45	0.45
1:A:199:ARG:NH2	1:A:201:GLN:HE21	2.10	0.45
1:A:208:PRO:HD2	1:A:209:TRP:CE3	2.51	0.45
1:A:43:THR:OG1	1:A:45:THR:HB	2.16	0.45
1:B:236:VAL:HG12	1:B:237:THR:N	2.31	0.45
1:B:293:ARG:NE	1:B:333:VAL:CG2	2.78	0.45
1:B:311:HIS:O	1:B:314:TYR:CE1	2.68	0.45
1:D:208:PRO:HD2	1:D:209:TRP:CE3	2.51	0.45
1:D:242:PHE:C	1:D:242:PHE:HD1	2.18	0.45
1:G:201:GLN:HG3	1:G:280:THR:CG2	2.24	0.45
1:H:117:LEU:HD21	1:H:133:PHE:HB2	1.98	0.45
1:H:55:TYR:CD1	1:H:223:ILE:HD11	2.51	0.45
1:A:238:LEU:HA	1:A:238:LEU:HD12	1.56	0.45
1:B:170:VAL:HB	1:B:178:ILE:HD11	1.99	0.45
1:B:252:ASN:OD1	1:B:254:GLN:N	2.49	0.45
1:D:43:THR:OG1	1:D:45:THR:HB	2.16	0.45
1:E:17:LEU:HA	1:E:152:LEU:HD21	1.99	0.45
1:F:117:LEU:HD21	1:F:133:PHE:HB2	1.98	0.45
1:F:242:PHE:HD1	1:F:242:PHE:C	2.18	0.45
1:G:242:PHE:HD1	1:G:242:PHE:C	2.18	0.45
1:G:293:ARG:NE	1:G:333:VAL:CG2	2.78	0.45
1:A:265:ARG:O	1:A:265:ARG:CG	2.64	0.45
1:C:79:ILE:CG2	1:G:124:MET:HG2	2.46	0.45
1:F:17:LEU:HA	1:F:152:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:GLN:HB2	1:G:67:TRP:CE2	2.51	0.45
1:B:290:ARG:NH2	1:B:307:HIS:CE1	2.85	0.45
1:C:290:ARG:NH2	1:C:307:HIS:CE1	2.85	0.45
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.62	0.45
1:A:211:LYS:NZ	1:E:232:GLY:O	2.40	0.45
1:F:316:LEU:HA	1:F:316:LEU:HD23	1.85	0.45
1:G:208:PRO:HD2	1:G:209:TRP:CE3	2.51	0.45
1:G:251:ASN:OD1	1:G:280:THR:CG2	2.59	0.45
1:H:236:VAL:HG12	1:H:237:THR:N	2.31	0.45
1:H:177:VAL:HA	1:H:304:GLU:O	2.16	0.45
1:C:144:TYR:HE2	1:C:319:HIS:NE2	2.13	0.45
1:D:17:LEU:HA	1:D:152:LEU:HD21	1.99	0.45
1:E:290:ARG:NH2	1:E:307:HIS:CE1	2.85	0.45
1:F:199:ARG:NH2	1:F:201:GLN:HE21	2.10	0.45
1:G:223:ILE:HB	1:G:224:TYR:HD1	1.67	0.45
1:B:117:LEU:CD2	1:B:133:PHE:HB2	2.47	0.45
1:B:69:GLN:CA	1:B:110:MET:HE1	2.46	0.45
1:G:290:ARG:NH2	1:G:307:HIS:CE1	2.85	0.45
1:H:290:ARG:NH2	1:H:307:HIS:CE1	2.85	0.45
1:A:290:ARG:NH2	1:A:307:HIS:CE1	2.85	0.45
1:B:17:LEU:HA	1:B:152:LEU:HD21	1.99	0.45
1:B:79:ILE:HD13	1:B:79:ILE:HA	1.78	0.45
1:C:97:LEU:HD11	1:C:125:PHE:CD2	2.52	0.45
1:D:270:LEU:HA	1:D:270:LEU:HD23	1.71	0.45
1:E:270:LEU:HD23	1:E:270:LEU:HA	1.71	0.45
1:F:102:VAL:HG13	1:F:103:PRO:CD	2.46	0.45
1:F:117:LEU:CD2	1:F:133:PHE:HB2	2.47	0.45
1:F:236:VAL:HG12	1:F:237:THR:N	2.31	0.45
1:H:43:THR:OG1	1:H:45:THR:HB	2.17	0.45
1:A:256:HIS:CE1	1:A:278:GLU:OE2	2.64	0.45
1:C:117:LEU:HD21	1:C:133:PHE:HB2	1.98	0.45
1:C:23:TYR:CD2	1:C:330:PHE:CE2	3.05	0.45
1:C:24:HIS:CD2	1:C:30:LEU:H	2.33	0.45
1:C:162:ARG:O	2:C:348:FAD:H2A	2.17	0.45
1:D:269:THR:HG23	1:D:269:THR:H	1.60	0.45
1:D:30:LEU:HD11	1:D:32:VAL:CG2	2.45	0.45
1:E:43:THR:OG1	1:E:45:THR:HB	2.17	0.45
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.70	0.45
1:A:270:LEU:HA	1:A:270:LEU:HD23	1.71	0.45
1:C:117:LEU:CD2	1:C:133:PHE:HB2	2.47	0.45
1:C:171:ALA:C	1:C:173:GLY:N	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:NH2	1:C:201:GLN:HE21	2.10	0.45
1:D:117:LEU:HD21	1:D:133:PHE:HB2	1.98	0.45
1:D:290:ARG:NH2	1:D:307:HIS:CE1	2.85	0.45
1:E:236:VAL:HG12	1:E:237:THR:N	2.31	0.45
1:G:117:LEU:CD2	1:G:133:PHE:HB2	2.47	0.45
1:G:324:LEU:HD23	1:G:324:LEU:HA	1.72	0.45
1:A:233:LEU:O	1:E:208:PRO:HB2	2.16	0.44
1:A:97:LEU:HD11	1:A:125:PHE:CD1	2.52	0.44
1:B:169:GLU:O	1:B:172:ARG:HB2	2.16	0.44
1:B:43:THR:OG1	1:B:45:THR:HB	2.17	0.44
1:D:195:LEU:HD12	1:D:195:LEU:HA	1.63	0.44
1:F:290:ARG:NH2	1:F:307:HIS:CE1	2.85	0.44
1:G:182:THR:OG1	1:G:186:ALA:HA	2.17	0.44
1:G:236:VAL:HG12	1:G:237:THR:N	2.31	0.44
1:H:17:LEU:HA	1:H:152:LEU:HD21	1.99	0.44
1:H:316:LEU:HD23	1:H:316:LEU:HA	1.85	0.44
1:H:61:ASN:HA	1:H:62:PRO:HD2	1.73	0.44
1:A:182:THR:OG1	1:A:186:ALA:HA	2.17	0.44
1:A:236:VAL:HG12	1:A:237:THR:N	2.31	0.44
1:B:133:PHE:CD1	1:B:134:ASN:N	2.86	0.44
1:B:58:GLU:HG2	1:B:106:TYR:HB3	1.99	0.44
1:C:133:PHE:CD1	1:C:134:ASN:N	2.86	0.44
1:C:184:VAL:HG23	1:C:185:TRP:CD2	2.53	0.44
1:E:184:VAL:HG23	1:E:185:TRP:CD2	2.53	0.44
1:G:30:LEU:CD1	1:G:31:ASP:N	2.67	0.44
1:G:43:THR:OG1	1:G:45:THR:HB	2.16	0.44
1:H:171:ALA:CB	1:H:298:PHE:CE2	3.00	0.44
1:A:133:PHE:CD1	1:A:134:ASN:N	2.86	0.44
1:C:17:LEU:HA	1:C:152:LEU:HD21	1.99	0.44
1:C:256:HIS:CE1	1:C:278:GLU:OE2	2.64	0.44
1:D:117:LEU:CD2	1:D:133:PHE:HB2	2.47	0.44
1:D:236:VAL:HG12	1:D:237:THR:N	2.31	0.44
1:F:182:THR:OG1	1:F:186:ALA:HA	2.18	0.44
1:F:62:PRO:C	1:F:64:GLU:N	2.67	0.44
1:A:218:ASP:OD1	1:A:219:LEU:N	2.50	0.44
1:D:182:THR:OG1	1:D:186:ALA:HA	2.17	0.44
1:F:184:VAL:HG23	1:F:185:TRP:CD2	2.53	0.44
1:G:59:PRO:HD3	1:G:106:TYR:CD1	2.52	0.44
1:G:122:LEU:HD23	1:G:122:LEU:HA	1.70	0.44
1:G:125:PHE:N	1:G:125:PHE:CD1	2.84	0.44
1:H:117:LEU:CD2	1:H:133:PHE:HB2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:256:HIS:CE1	1:H:278:GLU:OE2	2.64	0.44
1:A:201:GLN:HG3	1:A:280:THR:CG2	2.24	0.44
1:B:184:VAL:HG23	1:B:185:TRP:CD2	2.53	0.44
1:D:133:PHE:CD1	1:D:134:ASN:N	2.85	0.44
1:D:213:PHE:CD1	1:D:213:PHE:C	2.91	0.44
1:E:117:LEU:CD2	1:E:133:PHE:HB2	2.47	0.44
4:F:350:DTR:CD2	4:F:350:DTR:H	2.31	0.44
1:F:43:THR:OG1	1:F:45:THR:HB	2.16	0.44
1:G:196:GLN:O	1:G:285:VAL:HB	2.18	0.44
1:H:230:ILE:HA	1:H:231:PRO:HD2	1.75	0.44
1:A:117:LEU:CD2	1:A:133:PHE:HB2	2.47	0.44
1:B:196:GLN:O	1:B:285:VAL:HB	2.18	0.44
1:B:256:HIS:CB	1:E:42:PHE:HZ	2.30	0.44
1:E:133:PHE:CD1	1:E:134:ASN:N	2.85	0.44
1:E:213:PHE:C	1:E:213:PHE:CD1	2.91	0.44
1:E:279:TYR:CD1	1:E:279:TYR:N	2.86	0.44
1:F:213:PHE:CD1	1:F:213:PHE:C	2.91	0.44
1:G:162:ARG:O	2:G:348:FAD:H2A	2.18	0.44
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.86	0.44
1:B:167:PHE:CZ	1:B:189:LEU:HB3	2.53	0.44
1:D:55:TYR:CD1	1:D:224:TYR:OH	2.66	0.44
1:E:219:LEU:HD23	1:E:219:LEU:HA	1.73	0.44
1:H:279:TYR:CD1	1:H:279:TYR:N	2.86	0.44
1:H:2:ARG:HB2	1:H:176:ASP:OD2	2.18	0.44
1:A:265:ARG:O	1:A:265:ARG:HG2	2.17	0.44
1:B:246:ASN:C	1:B:246:ASN:OD1	2.57	0.44
1:C:246:ASN:C	1:C:246:ASN:OD1	2.56	0.44
1:D:177:VAL:HG12	1:D:178:ILE:N	2.24	0.44
1:D:223:ILE:HG23	1:D:223:ILE:O	2.18	0.44
1:F:167:PHE:CZ	1:F:189:LEU:HB3	2.53	0.44
1:G:238:LEU:HD12	1:G:238:LEU:HA	1.56	0.44
1:A:267:GLU:N	1:A:268:PRO:HD3	2.33	0.44
1:C:213:PHE:C	1:C:213:PHE:CD1	2.91	0.44
1:D:279:TYR:CD1	1:D:279:TYR:N	2.86	0.44
1:E:246:ASN:OD1	1:E:246:ASN:C	2.57	0.44
1:G:133:PHE:CD1	1:G:134:ASN:N	2.86	0.44
1:G:79:ILE:HD13	1:G:79:ILE:HA	1.78	0.44
1:H:167:PHE:CZ	1:H:189:LEU:HB3	2.53	0.44
1:H:213:PHE:CD1	1:H:213:PHE:C	2.91	0.44
1:B:269:THR:C	1:B:271:LYS:N	2.71	0.43
1:C:251:ASN:OD1	1:C:280:THR:CG2	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:VAL:HG23	1:D:185:TRP:CD2	2.53	0.43
1:E:167:PHE:CZ	1:E:189:LEU:HB3	2.53	0.43
1:E:196:GLN:O	1:E:285:VAL:HB	2.18	0.43
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.62	0.43
1:G:17:LEU:HA	1:G:152:LEU:HD21	1.99	0.43
1:G:216:THR:HG23	1:G:217:HIS:N	2.32	0.43
1:G:246:ASN:C	1:G:246:ASN:OD1	2.57	0.43
1:H:133:PHE:CD1	1:H:134:ASN:N	2.86	0.43
1:H:246:ASN:OD1	1:H:246:ASN:C	2.57	0.43
1:A:293:ARG:NH2	1:A:336:GLU:CD	2.61	0.43
1:C:23:TYR:O	1:C:30:LEU:CD2	2.66	0.43
1:C:279:TYR:CD1	1:C:279:TYR:N	2.86	0.43
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.80	0.43
1:D:196:GLN:O	1:D:285:VAL:HB	2.18	0.43
1:F:279:TYR:CD1	1:F:279:TYR:N	2.86	0.43
1:G:184:VAL:HG23	1:G:185:TRP:CD2	2.53	0.43
1:H:184:VAL:HG23	1:H:185:TRP:CD2	2.53	0.43
1:H:324:LEU:HD23	1:H:324:LEU:HA	1.72	0.43
1:A:22:ARG:CG	1:A:22:ARG:O	2.66	0.43
1:A:246:ASN:OD1	1:A:246:ASN:C	2.56	0.43
1:D:167:PHE:CZ	1:D:189:LEU:HB3	2.53	0.43
1:E:13:LEU:HD23	1:E:13:LEU:HA	1.62	0.43
1:F:196:GLN:O	1:F:285:VAL:HB	2.18	0.43
1:G:256:HIS:CE1	1:G:278:GLU:OE2	2.64	0.43
1:H:182:THR:OG1	1:H:186:ALA:HA	2.17	0.43
1:H:251:ASN:HA	1:H:280:THR:CG2	2.49	0.43
1:A:194:LEU:HA	1:A:194:LEU:HD23	1.08	0.43
1:C:182:THR:OG1	1:C:186:ALA:HA	2.17	0.43
1:C:167:PHE:CZ	1:C:189:LEU:HB3	2.53	0.43
1:D:267:GLU:N	1:D:268:PRO:HD3	2.33	0.43
1:G:152:LEU:HA	1:G:152:LEU:HD23	1.84	0.43
1:G:167:PHE:CZ	1:G:189:LEU:HB3	2.53	0.43
1:G:267:GLU:N	1:G:268:PRO:HD3	2.33	0.43
1:H:196:GLN:O	1:H:285:VAL:HB	2.18	0.43
1:A:196:GLN:O	1:A:285:VAL:HB	2.18	0.43
1:A:251:ASN:HA	1:A:280:THR:CG2	2.49	0.43
1:A:252:ASN:OD1	1:A:254:GLN:N	2.51	0.43
1:B:182:THR:OG1	1:B:186:ALA:HA	2.18	0.43
1:B:213:PHE:CD1	1:B:213:PHE:C	2.91	0.43
1:B:91:PRO:HA	1:B:137:LEU:HD23	2.01	0.43
1:C:251:ASN:HA	1:C:280:THR:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:256:HIS:CE1	1:D:278:GLU:OE2	2.64	0.43
1:D:251:ASN:HA	1:D:280:THR:CG2	2.49	0.43
1:E:170:VAL:CG1	1:E:178:ILE:HD13	2.48	0.43
1:E:58:GLU:CG	1:E:59:PRO:CD	2.96	0.43
1:F:133:PHE:CD1	1:F:134:ASN:N	2.86	0.43
1:H:250:ILE:HD12	1:H:250:ILE:HG23	1.44	0.43
1:A:17:LEU:HA	1:A:152:LEU:HD21	1.99	0.43
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.56	0.43
1:B:249:GLU:HB3	1:B:282:PHE:CE2	2.54	0.43
1:C:233:LEU:HD23	1:C:233:LEU:HA	1.74	0.43
1:D:250:ILE:HD12	1:D:250:ILE:HG23	1.44	0.43
1:E:152:LEU:HD23	1:E:152:LEU:HA	1.83	0.43
1:E:296:LEU:HD23	1:E:296:LEU:HA	1.50	0.43
1:H:148:LEU:HA	1:H:148:LEU:HD23	1.86	0.43
1:A:213:PHE:CD1	1:A:213:PHE:C	2.91	0.43
1:B:224:TYR:CG	1:B:242:PHE:HD2	2.36	0.43
1:C:76:LEU:HD23	1:C:76:LEU:HA	1.62	0.43
1:D:61:ASN:CB	1:D:63:GLN:HG3	2.43	0.43
1:D:90:THR:HG21	1:H:209:TRP:HD1	1.83	0.43
1:E:2:ARG:NH1	4:E:350:DTR:CD1	2.82	0.43
1:E:91:PRO:HA	1:E:137:LEU:HD23	2.01	0.43
1:F:62:PRO:O	1:F:63:GLN:C	2.55	0.43
1:G:249:GLU:HB3	1:G:282:PHE:CE2	2.54	0.43
1:H:175:ALA:O	1:H:303:THR:CG2	2.67	0.43
1:A:177:VAL:HG12	1:A:178:ILE:N	2.34	0.43
1:B:105:PRO:HD3	1:B:132:TRP:CE2	2.54	0.43
1:D:293:ARG:HD3	1:D:293:ARG:HH11	1.65	0.43
1:E:182:THR:OG1	1:E:186:ALA:HA	2.17	0.43
1:E:194:LEU:HA	1:E:194:LEU:HD23	1.08	0.43
1:E:252:ASN:OD1	1:E:255:ASP:N	2.43	0.43
1:F:105:PRO:HD3	1:F:132:TRP:CE2	2.54	0.43
1:H:91:PRO:HA	1:H:137:LEU:HD23	2.01	0.43
1:B:279:TYR:CD1	1:B:279:TYR:N	2.86	0.43
1:C:91:PRO:HA	1:C:137:LEU:HD23	2.01	0.43
1:C:215:ILE:HG22	1:C:217:HIS:CE1	2.54	0.43
1:D:27:LEU:HD21	1:D:334:LEU:HD13	1.99	0.43
1:D:79:ILE:HD13	1:D:79:ILE:HA	1.78	0.43
1:H:35:TYR:HE1	1:H:160:PHE:CD2	2.37	0.43
1:A:167:PHE:CZ	1:A:189:LEU:HB3	2.53	0.43
1:B:267:GLU:N	1:B:268:PRO:HD3	2.33	0.43
1:B:269:THR:H	1:B:269:THR:HG23	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:VAL:CG1	1:D:178:ILE:N	2.75	0.43
1:D:324:LEU:HA	1:D:324:LEU:HD23	1.72	0.43
1:D:35:TYR:HE1	1:D:160:PHE:CD2	2.37	0.43
1:D:91:PRO:HA	1:D:137:LEU:HD23	2.01	0.43
1:E:293:ARG:HH11	1:E:293:ARG:HD3	1.65	0.43
1:F:249:GLU:HB3	1:F:282:PHE:CE2	2.54	0.43
1:G:230:ILE:HA	1:G:231:PRO:HD2	1.75	0.43
1:A:253:ILE:CG1	1:F:42:PHE:CG	2.95	0.42
1:B:35:TYR:HE1	1:B:160:PHE:CD2	2.37	0.42
1:C:97:LEU:HB3	1:C:128:TYR:CG	2.54	0.42
1:D:13:LEU:HD23	1:D:13:LEU:HA	1.62	0.42
1:D:246:ASN:OD1	1:D:246:ASN:C	2.57	0.42
1:F:246:ASN:C	1:F:246:ASN:OD1	2.57	0.42
1:F:49:ALA:HB3	2:F:348:FAD:O4	2.20	0.42
1:H:170:VAL:HG12	1:H:175:ALA:HB2	2.01	0.42
1:H:249:GLU:HB3	1:H:282:PHE:CE2	2.54	0.42
1:A:91:PRO:HA	1:A:137:LEU:HD23	2.01	0.42
1:A:152:LEU:HA	1:A:152:LEU:HD23	1.84	0.42
1:A:184:VAL:HG23	1:A:185:TRP:CD2	2.53	0.42
1:C:196:GLN:O	1:C:285:VAL:HB	2.18	0.42
1:C:249:GLU:HB3	1:C:282:PHE:CE2	2.54	0.42
1:D:233:LEU:HD23	1:D:233:LEU:HA	1.74	0.42
1:E:35:TYR:HE1	1:E:160:PHE:CD2	2.37	0.42
1:G:251:ASN:HA	1:G:280:THR:CG2	2.49	0.42
1:H:229:ILE:C	1:H:230:ILE:HG13	2.39	0.42
1:H:267:GLU:N	1:H:268:PRO:HD3	2.33	0.42
1:A:331:GLY:O	1:A:335:GLU:N	2.50	0.42
1:B:124:MET:HE2	1:F:112:LEU:HD13	2.01	0.42
1:B:52:TRP:O	1:B:52:TRP:HE3	2.03	0.42
1:C:105:PRO:HD3	1:C:132:TRP:CE2	2.54	0.42
1:E:238:LEU:HA	1:E:238:LEU:HD12	1.56	0.42
1:E:249:GLU:HB3	1:E:282:PHE:CE2	2.54	0.42
1:E:331:GLY:O	1:E:335:GLU:N	2.50	0.42
1:H:102:VAL:HG13	1:H:103:PRO:CD	2.46	0.42
1:A:229:ILE:C	1:A:230:ILE:HG13	2.40	0.42
1:A:279:TYR:CD1	1:A:279:TYR:N	2.86	0.42
1:B:52:TRP:CZ3	1:B:54:PRO:HD3	2.55	0.42
1:C:35:TYR:HE1	1:C:160:PHE:CD2	2.37	0.42
1:D:170:VAL:HG12	1:D:178:ILE:HD11	2.00	0.42
1:D:223:ILE:O	1:D:223:ILE:CG2	2.67	0.42
1:D:249:GLU:HB3	1:D:282:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:52:TRP:HE3	1:D:52:TRP:O	2.03	0.42
1:E:102:VAL:HG13	1:E:103:PRO:CD	2.46	0.42
1:E:105:PRO:HD3	1:E:132:TRP:CE2	2.54	0.42
1:E:251:ASN:HA	1:E:280:THR:CG2	2.49	0.42
1:G:69:GLN:CA	1:G:110:MET:HE2	2.50	0.42
1:H:233:LEU:HD23	1:H:233:LEU:HA	1.74	0.42
1:A:49:ALA:HB3	2:A:348:FAD:O4	2.20	0.42
1:C:229:ILE:C	1:C:230:ILE:HG13	2.40	0.42
1:C:267:GLU:N	1:C:268:PRO:HD3	2.33	0.42
1:C:52:TRP:HE3	1:C:52:TRP:O	2.03	0.42
1:E:230:ILE:HA	1:E:231:PRO:HD2	1.75	0.42
1:E:267:GLU:N	1:E:268:PRO:HD3	2.33	0.42
1:E:52:TRP:CZ3	1:E:54:PRO:HD3	2.55	0.42
1:F:138:ILE:HG21	1:F:138:ILE:HD13	1.72	0.42
1:F:251:ASN:HA	1:F:280:THR:CG2	2.49	0.42
1:F:267:GLU:N	1:F:268:PRO:HD3	2.33	0.42
1:F:52:TRP:CZ3	1:F:54:PRO:HD3	2.55	0.42
1:G:177:VAL:CG1	1:G:178:ILE:N	2.82	0.42
1:G:279:TYR:N	1:G:279:TYR:CD1	2.86	0.42
1:B:13:LEU:HD23	1:B:13:LEU:HA	1.61	0.42
1:D:219:LEU:HA	1:D:219:LEU:HD23	1.63	0.42
1:D:219:LEU:N	1:D:219:LEU:HD23	2.27	0.42
1:G:213:PHE:CD1	1:G:213:PHE:C	2.91	0.42
1:H:105:PRO:HD3	1:H:132:TRP:CE2	2.54	0.42
1:H:52:TRP:HE3	1:H:52:TRP:O	2.03	0.42
1:A:35:TYR:HE1	1:A:160:PHE:CD2	2.37	0.42
1:B:101:ALA:HA	1:B:130:TYR:CD2	2.55	0.42
1:B:229:ILE:C	1:B:230:ILE:HG13	2.40	0.42
1:C:52:TRP:CZ3	1:C:54:PRO:HD3	2.55	0.42
1:G:39:PHE:O	1:G:42:PHE:N	2.42	0.42
1:H:52:TRP:CZ3	1:H:54:PRO:HD3	2.55	0.42
1:H:79:ILE:HD13	1:H:79:ILE:HA	1.78	0.42
1:A:118:THR:H	1:A:118:THR:HG23	1.56	0.42
1:C:168:GLU:HA	1:C:171:ALA:HB3	2.01	0.42
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.56	0.42
1:D:265:ARG:NH1	1:D:265:ARG:CG	2.80	0.42
1:E:101:ALA:HA	1:E:130:TYR:CD2	2.55	0.42
1:E:250:ILE:HG23	1:E:250:ILE:HD12	1.44	0.42
1:G:293:ARG:HD3	1:G:293:ARG:HH11	1.65	0.42
1:H:101:ALA:HA	1:H:130:TYR:CD2	2.55	0.42
1:H:170:VAL:HG12	1:H:175:ALA:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.55	0.42
1:A:170:VAL:HG12	1:A:175:ALA:HB2	2.02	0.42
1:A:249:GLU:HB3	1:A:282:PHE:CE2	2.54	0.42
1:D:102:VAL:HG13	1:D:103:PRO:CD	2.46	0.42
1:D:177:VAL:HG22	1:D:304:GLU:HB2	2.02	0.42
1:D:229:ILE:C	1:D:230:ILE:HG13	2.40	0.42
1:F:52:TRP:HE3	1:F:52:TRP:O	2.02	0.42
1:G:91:PRO:HA	1:G:137:LEU:HD23	2.01	0.42
1:A:133:PHE:C	1:A:133:PHE:CD1	2.93	0.42
1:A:314:TYR:N	1:A:314:TYR:CD1	2.87	0.42
1:A:52:TRP:O	1:A:52:TRP:HE3	2.03	0.42
1:B:251:ASN:HA	1:B:280:THR:CG2	2.49	0.42
1:C:101:ALA:HA	1:C:130:TYR:CD2	2.55	0.42
1:D:101:ALA:HA	1:D:130:TYR:CD2	2.55	0.42
1:D:105:PRO:HD3	1:D:132:TRP:CE2	2.54	0.42
1:D:218:ASP:HB2	1:D:226:SER:OG	2.20	0.42
1:D:293:ARG:NH2	1:D:336:GLU:CD	2.61	0.42
1:D:49:ALA:HB3	2:D:348:FAD:O4	2.20	0.42
1:E:49:ALA:HB3	2:E:348:FAD:O4	2.20	0.42
1:F:101:ALA:HA	1:F:130:TYR:CD2	2.55	0.42
1:F:133:PHE:CD1	1:F:133:PHE:C	2.94	0.42
1:F:35:TYR:HE1	1:F:160:PHE:CD2	2.37	0.42
1:F:217:HIS:CD2	5:F:363:HOH:O	2.73	0.42
1:F:229:ILE:C	1:F:230:ILE:HG13	2.40	0.42
1:G:35:TYR:HE1	1:G:160:PHE:CD2	2.37	0.42
1:H:176:ASP:C	1:H:177:VAL:HG23	2.39	0.42
1:H:59:PRO:HG3	1:H:65:ALA:HB2	2.02	0.42
1:A:13:LEU:HA	1:A:13:LEU:HD23	1.61	0.41
1:B:119:PRO:CD	5:B:356:HOH:O	2.68	0.41
1:F:324:LEU:HA	1:F:324:LEU:HD23	1.72	0.41
1:H:122:LEU:O	1:H:124:MET:N	2.53	0.41
1:H:172:ARG:O	1:H:174:GLY:N	2.45	0.41
1:C:133:PHE:CD1	1:C:133:PHE:C	2.93	0.41
1:C:49:ALA:HB3	2:C:348:FAD:O4	2.20	0.41
1:D:133:PHE:CD1	1:D:133:PHE:C	2.93	0.41
1:D:147:TRP:CE2	1:D:151:ARG:HD3	2.56	0.41
1:G:101:ALA:HA	1:G:130:TYR:CD2	2.55	0.41
1:G:102:VAL:HG21	1:G:219:LEU:HD21	2.02	0.41
1:G:229:ILE:C	1:G:230:ILE:HG13	2.40	0.41
1:G:43:THR:HG23	1:G:43:THR:H	1.66	0.41
1:H:49:ALA:HB3	2:H:348:FAD:O4	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ILE:HA	1:A:231:PRO:HD2	1.75	0.41
1:C:13:LEU:HD23	1:C:13:LEU:HA	1.62	0.41
1:F:76:LEU:HD23	1:F:76:LEU:HA	1.62	0.41
1:G:52:TRP:HE3	1:G:52:TRP:O	2.03	0.41
1:H:122:LEU:O	1:H:125:PHE:N	2.41	0.41
1:H:133:PHE:C	1:H:133:PHE:CD1	2.94	0.41
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.86	0.41
1:C:324:LEU:HD23	1:C:324:LEU:HA	1.72	0.41
1:E:133:PHE:CD1	1:E:133:PHE:C	2.93	0.41
1:F:145:LEU:HD23	1:F:145:LEU:HA	1.80	0.41
1:F:216:THR:CG2	1:F:217:HIS:N	2.80	0.41
1:F:91:PRO:HA	1:F:137:LEU:HD23	2.01	0.41
1:G:105:PRO:HD3	1:G:132:TRP:CE2	2.54	0.41
1:G:147:TRP:CE2	1:G:151:ARG:HD3	2.56	0.41
1:G:270:LEU:HD23	1:G:270:LEU:HA	1.71	0.41
1:H:2:ARG:NH2	1:H:174:GLY:HA3	2.35	0.41
1:D:223:ILE:CB	1:D:224:TYR:CD1	3.01	0.41
1:D:52:TRP:CZ3	1:D:54:PRO:HD3	2.55	0.41
1:E:233:LEU:HD23	1:E:233:LEU:HA	1.74	0.41
1:E:52:TRP:HE3	1:E:52:TRP:O	2.03	0.41
1:F:43:THR:HG23	1:F:43:THR:H	1.66	0.41
1:B:133:PHE:CD1	1:B:133:PHE:C	2.93	0.41
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.80	0.41
1:B:201:GLN:HG3	1:B:280:THR:CG2	2.24	0.41
1:F:147:TRP:CE2	1:F:151:ARG:HD3	2.56	0.41
1:G:49:ALA:HB3	2:G:348:FAD:O4	2.19	0.41
1:G:52:TRP:CZ3	1:G:54:PRO:HD3	2.55	0.41
1:H:252:ASN:OD1	1:H:255:ASP:N	2.43	0.41
1:H:270:LEU:C	1:H:272:ASP:N	2.74	0.41
1:A:147:TRP:CE2	1:A:151:ARG:HD3	2.56	0.41
1:A:316:LEU:HB2	2:A:348:FAD:O2	2.21	0.41
1:A:52:TRP:CZ3	1:A:54:PRO:HD3	2.55	0.41
1:B:331:GLY:O	1:B:335:GLU:N	2.49	0.41
1:C:102:VAL:HG13	1:C:103:PRO:CD	2.46	0.41
1:C:250:ILE:HD12	1:C:250:ILE:HG23	1.44	0.41
1:D:30:LEU:C	1:D:30:LEU:CD1	2.72	0.41
1:D:316:LEU:HB2	2:D:348:FAD:O2	2.21	0.41
1:E:195:LEU:HD12	1:E:195:LEU:HA	1.63	0.41
1:F:195:LEU:HA	1:F:195:LEU:HD12	1.63	0.41
1:F:55:TYR:HE1	1:F:224:TYR:HH	1.61	0.41
1:F:48:ALA:HB1	2:F:348:FAD:C4X	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:316:LEU:HB2	2:G:348:FAD:O2	2.21	0.41
1:A:270:LEU:C	1:A:272:ASP:N	2.74	0.41
1:B:128:TYR:HD1	1:B:128:TYR:H	1.69	0.41
1:B:147:TRP:CE2	1:B:151:ARG:HD3	2.56	0.41
1:B:160:PHE:CB	1:B:162:ARG:HG3	2.51	0.41
1:B:253:ILE:HA	1:E:42:PHE:CZ	2.54	0.41
1:B:49:ALA:HB3	2:B:348:FAD:O4	2.19	0.41
1:E:118:THR:HG23	1:E:118:THR:H	1.56	0.41
1:E:229:ILE:C	1:E:230:ILE:HG13	2.40	0.41
1:F:270:LEU:C	1:F:272:ASP:N	2.74	0.41
1:G:270:LEU:C	1:G:272:ASP:N	2.74	0.41
1:G:48:ALA:HB1	2:G:348:FAD:C4X	2.51	0.41
1:H:40:THR:OG1	1:H:142:ARG:NH1	2.53	0.41
1:B:126:PRO:HD2	5:B:351:HOH:O	2.19	0.41
1:B:195:LEU:HA	1:B:195:LEU:HD12	1.63	0.41
1:C:270:LEU:C	1:C:272:ASP:N	2.74	0.41
1:D:152:LEU:HD23	1:D:152:LEU:HA	1.83	0.41
1:H:147:TRP:CE2	1:H:151:ARG:HD3	2.56	0.41
1:H:316:LEU:HB2	2:H:348:FAD:O2	2.21	0.41
1:A:268:PRO:HB2	1:E:82:PRO:CA	2.45	0.41
1:A:26:VAL:HG12	1:A:26:VAL:O	2.21	0.41
1:A:48:ALA:HB1	2:A:348:FAD:C4X	2.51	0.41
1:B:152:LEU:HD23	1:B:152:LEU:HA	1.84	0.41
1:B:55:TYR:HD1	1:B:55:TYR:H	1.68	0.41
1:C:145:LEU:HA	1:C:145:LEU:HD23	1.80	0.41
1:C:147:TRP:CE2	1:C:151:ARG:HD3	2.56	0.41
1:C:152:LEU:HD23	1:C:152:LEU:HA	1.84	0.41
1:C:175:ALA:O	1:C:303:THR:HG22	2.21	0.41
1:C:316:LEU:HD23	1:C:316:LEU:HA	1.85	0.41
1:E:30:LEU:C	1:E:30:LEU:HD12	2.41	0.41
1:F:24:HIS:HB3	5:F:368:HOH:O	2.21	0.41
1:G:102:VAL:HG13	1:G:103:PRO:CD	2.45	0.41
1:G:224:TYR:CG	1:G:242:PHE:HD2	2.38	0.41
1:A:269:THR:H	1:A:269:THR:HG23	1.60	0.41
1:A:51:LEU:HD23	1:A:215:ILE:HD11	2.03	0.41
1:B:233:LEU:HD23	1:B:233:LEU:HA	1.74	0.41
1:C:195:LEU:HD22	1:C:309:TYR:CE1	2.56	0.41
1:C:48:ALA:HB1	2:C:348:FAD:C4X	2.51	0.41
1:E:98:PHE:O	1:E:128:TYR:HB3	2.21	0.41
1:F:122:LEU:HD23	1:F:122:LEU:HA	1.70	0.41
1:H:48:ALA:HB1	2:H:348:FAD:C4X	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:LEU:HD22	1:A:309:TYR:CE1	2.56	0.40
1:B:122:LEU:HA	1:B:122:LEU:HD23	1.70	0.40
1:B:250:ILE:HD12	1:B:250:ILE:HG23	1.44	0.40
1:D:48:ALA:HB1	2:D:348:FAD:C4X	2.51	0.40
1:E:147:TRP:CE2	1:E:151:ARG:HD3	2.56	0.40
1:E:195:LEU:HD22	1:E:309:TYR:CE1	2.56	0.40
1:F:233:LEU:HD23	1:F:233:LEU:HA	1.74	0.40
1:H:89:LEU:O	1:H:90:THR:HG23	2.22	0.40
1:A:105:PRO:HD3	1:A:132:TRP:CE2	2.54	0.40
1:B:102:VAL:HG13	1:B:103:PRO:CD	2.46	0.40
1:B:253:ILE:HD12	1:B:253:ILE:HG21	1.87	0.40
1:D:55:TYR:CE1	1:D:314:TYR:HD1	2.39	0.40
1:E:10:VAL:O	1:E:14:SER:OG	2.39	0.40
1:E:269:THR:HG23	1:E:269:THR:H	1.60	0.40
1:F:223:ILE:CG1	1:F:224:TYR:CE1	3.00	0.40
1:F:62:PRO:O	1:F:64:GLU:N	2.54	0.40
1:F:63:GLN:H	1:F:63:GLN:HG3	1.63	0.40
1:G:118:THR:H	1:G:118:THR:HG23	1.56	0.40
1:G:133:PHE:C	1:G:133:PHE:CD1	2.93	0.40
1:G:311:HIS:O	1:G:314:TYR:CD1	2.74	0.40
1:G:76:LEU:HD23	1:G:76:LEU:HA	1.61	0.40
1:A:69:GLN:CA	1:A:110:MET:HE2	2.51	0.40
1:B:195:LEU:HD22	1:B:309:TYR:CE1	2.56	0.40
1:C:118:THR:CB	1:C:119:PRO:CD	3.00	0.40
1:C:165:GLU:HB2	1:C:169:GLU:OE2	2.21	0.40
1:C:22:ARG:CG	1:C:23:TYR:CE1	3.04	0.40
1:D:195:LEU:HD22	1:D:309:TYR:CE1	2.56	0.40
1:D:331:GLY:O	1:D:335:GLU:N	2.49	0.40
1:F:316:LEU:HB2	2:F:348:FAD:O2	2.21	0.40
1:G:165:GLU:HB2	1:G:169:GLU:OE2	2.20	0.40
1:G:195:LEU:HD22	1:G:309:TYR:CE1	2.56	0.40
1:A:118:THR:CB	1:A:119:PRO:CD	3.00	0.40
1:A:22:ARG:HG2	1:A:23:TYR:CD1	2.56	0.40
1:B:48:ALA:HB1	2:B:348:FAD:C4X	2.51	0.40
1:B:89:LEU:O	1:B:90:THR:HG23	2.21	0.40
1:C:238:LEU:HA	1:C:238:LEU:HD12	1.56	0.40
1:B:256:HIS:CB	1:E:42:PHE:CZ	3.05	0.40
1:G:195:LEU:HA	1:G:195:LEU:HD12	1.63	0.40
1:G:89:LEU:O	1:G:90:THR:HG23	2.22	0.40
1:H:118:THR:CB	1:H:119:PRO:CD	3.00	0.40
1:H:172:ARG:C	1:H:174:GLY:N	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:195:LEU:HD22	1:H:309:TYR:CE1	2.56	0.40
1:B:270:LEU:C	1:B:272:ASP:N	2.74	0.40
1:C:177:VAL:HA	1:C:304:GLU:O	2.21	0.40
1:C:241:THR:N	5:C:357:HOH:O	2.20	0.40
1:C:51:LEU:HD23	1:C:215:ILE:HD11	2.03	0.40
1:F:288:GLN:HE21	1:F:288:GLN:HB2	1.26	0.40
1:G:194:LEU:HD23	1:G:194:LEU:HA	1.08	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:ASP:OD1	1:H:162:ARG:NH2[4_565]	2.01	0.19
1:A:332:LYS:NZ	1:D:126:PRO:CG[7_545]	2.11	0.09
1:C:123:ASP:OD2	1:H:35:TYR:OH[4_565]	2.15	0.05
1:C:162:ARG:NH2	1:H:123:ASP:OD1[3_655]	2.17	0.03

## 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	337/347 (97%)	310 (92%)	25 (7%)	2 (1%)	25 59
1	B	337/347 (97%)	309 (92%)	25 (7%)	3 (1%)	17 52
1	C	337/347 (97%)	312 (93%)	23 (7%)	2 (1%)	25 59
1	D	337/347 (97%)	309 (92%)	25 (7%)	3 (1%)	17 52
1	E	337/347 (97%)	309 (92%)	25 (7%)	3 (1%)	17 52
1	F	337/347 (97%)	311 (92%)	24 (7%)	2 (1%)	25 59
1	G	337/347 (97%)	306 (91%)	27 (8%)	4 (1%)	13 44
1	H	337/347 (97%)	310 (92%)	23 (7%)	4 (1%)	13 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2696/2776 (97%)	2476 (92%)	197 (7%)	23 (1%)	17	52

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	28	GLN
1	E	28	GLN
1	A	28	GLN
1	B	24	HIS
1	G	222	GLY
1	A	240	GLY
1	B	240	GLY
1	C	240	GLY
1	D	240	GLY
1	E	29	PRO
1	E	240	GLY
1	F	221	ARG
1	F	240	GLY
1	G	240	GLY
1	H	123	ASP
1	H	240	GLY
1	H	271	LYS
1	B	271	LYS
1	D	29	PRO
1	D	126	PRO
1	G	26	VAL
1	H	173	GLY
1	G	29	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/298 (97%)	263 (91%)	27 (9%)	9	32
1	B	290/298 (97%)	265 (91%)	25 (9%)	10	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	290/298 (97%)	266 (92%)	24 (8%)	11	38
1	D	290/298 (97%)	265 (91%)	25 (9%)	10	37
1	E	290/298 (97%)	263 (91%)	27 (9%)	9	32
1	F	290/298 (97%)	263 (91%)	27 (9%)	9	32
1	G	290/298 (97%)	263 (91%)	27 (9%)	9	32
1	H	290/298 (97%)	268 (92%)	22 (8%)	13	41
All	All	2320/2384 (97%)	2116 (91%)	204 (9%)	10	36

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	SER
1	A	17	LEU
1	A	28	GLN
1	A	30	LEU
1	A	31	ASP
1	A	60	SER
1	A	61	ASN
1	A	76	LEU
1	A	89	LEU
1	A	99	ARG
1	A	138	ILE
1	A	142	ARG
1	A	151	ARG
1	A	184	VAL
1	A	190	GLN
1	A	205	VAL
1	A	216	THR
1	A	221	ARG
1	A	224	TYR
1	A	238	LEU
1	A	242	PHE
1	A	252	ASN
1	A	253	ILE
1	A	254	GLN
1	A	258	THR
1	A	276	VAL
1	A	291	LEU
1	B	14	SER
1	B	17	LEU

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Mol	Chain	Res	Type
1	B	22	ARG
1	B	55	TYR
1	B	56	THR
1	B	76	LEU
1	B	89	LEU
1	B	99	ARG
1	B	128	TYR
1	B	138	ILE
1	B	142	ARG
1	B	151	ARG
1	B	184	VAL
1	B	190	GLN
1	B	205	VAL
1	B	216	THR
1	B	224	TYR
1	B	238	LEU
1	B	242	PHE
1	B	252	ASN
1	B	253	ILE
1	B	258	THR
1	B	265	ARG
1	B	276	VAL
1	B	291	LEU
1	C	14	SER
1	C	17	LEU
1	C	28	GLN
1	C	29	PRO
1	C	76	LEU
1	C	89	LEU
1	C	99	ARG
1	C	129	ARG
1	C	138	ILE
1	C	142	ARG
1	C	151	ARG
1	C	184	VAL
1	C	190	GLN
1	C	205	VAL
1	C	216	THR
1	C	224	TYR
1	C	238	LEU
1	C	242	PHE
1	C	252	ASN

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Mol	Chain	Res	Type
1	C	253	ILE
1	C	258	THR
1	C	276	VAL
1	C	288	GLN
1	C	291	LEU
1	D	14	SER
1	D	17	LEU
1	D	22	ARG
1	D	24	HIS
1	D	30	LEU
1	D	61	ASN
1	D	76	LEU
1	D	89	LEU
1	D	99	ARG
1	D	138	ILE
1	D	142	ARG
1	D	151	ARG
1	D	162	ARG
1	D	184	VAL
1	D	190	GLN
1	D	205	VAL
1	D	216	THR
1	D	224	TYR
1	D	238	LEU
1	D	242	PHE
1	D	252	ASN
1	D	253	ILE
1	D	258	THR
1	D	276	VAL
1	D	291	LEU
1	E	14	SER
1	E	17	LEU
1	E	22	ARG
1	E	57	SER
1	E	58	GLU
1	E	61	ASN
1	E	76	LEU
1	E	89	LEU
1	E	99	ARG
1	E	125	PHE
1	E	138	ILE
1	E	142	ARG

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Mol	Chain	Res	Type
1	E	151	ARG
1	E	184	VAL
1	E	190	GLN
1	E	205	VAL
1	E	216	THR
1	E	223	ILE
1	E	224	TYR
1	E	225	ASN
1	E	238	LEU
1	E	242	PHE
1	E	252	ASN
1	E	253	ILE
1	E	258	THR
1	E	276	VAL
1	E	291	LEU
1	F	14	SER
1	F	17	LEU
1	F	22	ARG
1	F	60	SER
1	F	62	PRO
1	F	76	LEU
1	F	89	LEU
1	F	99	ARG
1	F	138	ILE
1	F	142	ARG
1	F	151	ARG
1	F	184	VAL
1	F	190	GLN
1	F	205	VAL
1	F	216	THR
1	F	219	LEU
1	F	224	TYR
1	F	225	ASN
1	F	238	LEU
1	F	242	PHE
1	F	252	ASN
1	F	253	ILE
1	F	254	GLN
1	F	258	THR
1	F	276	VAL
1	F	288	GLN
1	F	291	LEU

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Mol	Chain	Res	Type
1	G	14	SER
1	G	17	LEU
1	G	30	LEU
1	G	56	THR
1	G	63	GLN
1	G	76	LEU
1	G	89	LEU
1	G	99	ARG
1	G	125	PHE
1	G	138	ILE
1	G	142	ARG
1	G	151	ARG
1	G	184	VAL
1	G	190	GLN
1	G	205	VAL
1	G	216	THR
1	G	218	ASP
1	G	223	ILE
1	G	224	TYR
1	G	225	ASN
1	G	238	LEU
1	G	242	PHE
1	G	252	ASN
1	G	253	ILE
1	G	258	THR
1	G	276	VAL
1	G	291	LEU
1	H	14	SER
1	H	17	LEU
1	H	28	GLN
1	H	76	LEU
1	H	89	LEU
1	H	99	ARG
1	H	129	ARG
1	H	138	ILE
1	H	142	ARG
1	H	151	ARG
1	H	184	VAL
1	H	190	GLN
1	H	205	VAL
1	H	216	THR
1	H	224	TYR

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Mol	Chain	Res	Type
1	H	238	LEU
1	H	242	PHE
1	H	252	ASN
1	H	253	ILE
1	H	258	THR
1	H	276	VAL
1	H	291	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	61	ASN
1	A	63	GLN
1	A	201	GLN
1	A	217	HIS
1	A	307	HIS
1	B	53	GLN
1	B	96	ASN
1	B	201	GLN
1	B	217	HIS
1	B	288	GLN
1	B	307	HIS
1	C	24	HIS
1	C	53	GLN
1	C	96	ASN
1	C	201	GLN
1	C	217	HIS
1	C	288	GLN
1	C	307	HIS
1	D	24	HIS
1	D	53	GLN
1	D	63	GLN
1	D	86	ASN
1	D	96	ASN
1	D	201	GLN
1	D	217	HIS
1	D	225	ASN
1	D	288	GLN
1	D	307	HIS
1	E	53	GLN
1	E	96	ASN

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Mol	Chain	Res	Type
1	E	201	GLN
1	E	217	HIS
1	E	307	HIS
1	F	201	GLN
1	F	217	HIS
1	F	254	GLN
1	F	288	GLN
1	F	307	HIS
1	G	53	GLN
1	G	96	ASN
1	G	201	GLN
1	G	217	HIS
1	G	307	HIS
1	H	53	GLN
1	H	96	ASN
1	H	201	GLN
1	H	217	HIS
1	H	307	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	FAD	G	348	-	51,58,58	1.17	4 (7%)	60,89,89	2.48	13 (21%)
3	ITR	H	349	-	13,16,16	1.03	1 (7%)	11,22,22	1.09	1 (9%)
2	FAD	E	348	-	51,58,58	1.17	4 (7%)	60,89,89	2.48	13 (21%)
2	FAD	A	348	-	51,58,58	1.16	4 (7%)	60,89,89	2.48	13 (21%)
3	ITR	D	349	-	13,16,16	1.04	1 (7%)	11,22,22	1.09	1 (9%)
2	FAD	B	348	-	51,58,58	1.17	4 (7%)	60,89,89	2.48	13 (21%)
3	ITR	B	349	-	13,16,16	1.03	1 (7%)	11,22,22	1.09	1 (9%)
2	FAD	F	348	-	51,58,58	1.16	5 (9%)	60,89,89	2.48	13 (21%)
2	FAD	D	348	-	51,58,58	1.17	5 (9%)	60,89,89	2.49	13 (21%)
3	ITR	F	349	-	13,16,16	1.04	1 (7%)	11,22,22	1.08	1 (9%)
3	ITR	A	349	-	13,16,16	1.04	1 (7%)	11,22,22	1.09	1 (9%)
2	FAD	H	348	-	51,58,58	1.17	4 (7%)	60,89,89	2.48	13 (21%)
3	ITR	E	349	-	13,16,16	1.04	1 (7%)	11,22,22	1.09	1 (9%)
2	FAD	C	348	-	51,58,58	1.16	4 (7%)	60,89,89	2.48	13 (21%)
3	ITR	G	349	-	13,16,16	1.04	1 (7%)	11,22,22	1.09	1 (9%)
3	ITR	C	349	-	13,16,16	1.03	1 (7%)	11,22,22	1.08	1 (9%)

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	G	348	-	-	5/30/50/50	0/6/6/6
3	ITR	H	349	-	-	0/3/8/8	0/2/2/2
2	FAD	E	348	-	-	5/30/50/50	0/6/6/6
2	FAD	A	348	-	-	5/30/50/50	0/6/6/6
3	ITR	D	349	-	-	0/3/8/8	0/2/2/2
2	FAD	B	348	-	-	5/30/50/50	0/6/6/6
3	ITR	B	349	-	-	0/3/8/8	0/2/2/2
2	FAD	F	348	-	-	5/30/50/50	0/6/6/6
2	FAD	D	348	-	-	5/30/50/50	0/6/6/6
3	ITR	F	349	-	-	0/3/8/8	0/2/2/2
3	ITR	A	349	-	-	0/3/8/8	0/2/2/2
2	FAD	H	348	-	-	5/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ITR	E	349	-	-	0/3/8/8	0/2/2/2
2	FAD	C	348	-	-	5/30/50/50	0/6/6/6
3	ITR	G	349	-	-	0/3/8/8	0/2/2/2
3	ITR	C	349	-	-	0/3/8/8	0/2/2/2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	348	FAD	C4-N3	3.66	1.39	1.33
2	C	348	FAD	C4-N3	3.66	1.39	1.33
2	B	348	FAD	C4-N3	3.64	1.39	1.33
2	E	348	FAD	C4-N3	3.64	1.39	1.33
2	D	348	FAD	C4-N3	3.64	1.39	1.33
2	G	348	FAD	C4-N3	3.63	1.39	1.33
2	F	348	FAD	C4-N3	3.63	1.39	1.33
2	A	348	FAD	C4-N3	3.62	1.39	1.33
2	C	348	FAD	C2-N1	-2.84	1.32	1.38
2	H	348	FAD	C2-N1	-2.83	1.32	1.38
2	D	348	FAD	C2-N1	-2.83	1.32	1.38
2	A	348	FAD	C2-N1	-2.82	1.32	1.38
2	B	348	FAD	C2-N1	-2.82	1.32	1.38
2	E	348	FAD	C2-N1	-2.81	1.32	1.38
2	F	348	FAD	C2-N1	-2.81	1.32	1.38
2	G	348	FAD	C2-N1	-2.80	1.32	1.38
2	G	348	FAD	C4X-C10	2.60	1.41	1.38
2	H	348	FAD	C4X-C10	2.50	1.41	1.38
2	C	348	FAD	C4X-C10	2.49	1.41	1.38
2	E	348	FAD	C4X-C10	2.49	1.41	1.38
2	D	348	FAD	C4X-C10	2.48	1.41	1.38
2	B	348	FAD	C10-N1	2.46	1.36	1.33
2	B	348	FAD	C4X-C10	2.44	1.41	1.38
2	A	348	FAD	C10-N1	2.43	1.36	1.33
2	F	348	FAD	C4X-C10	2.42	1.41	1.38
2	A	348	FAD	C4X-C10	2.41	1.41	1.38
2	D	348	FAD	C10-N1	2.40	1.36	1.33
2	F	348	FAD	C10-N1	2.39	1.36	1.33
2	C	348	FAD	C10-N1	2.38	1.36	1.33
2	E	348	FAD	C10-N1	2.38	1.36	1.33
2	H	348	FAD	C10-N1	2.37	1.36	1.33
2	G	348	FAD	C10-N1	2.33	1.36	1.33
3	E	349	ITR	CA-N	2.13	1.32	1.27
3	G	349	ITR	CA-N	2.12	1.32	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	349	ITR	CA-N	2.09	1.32	1.27
3	C	349	ITR	CA-N	2.09	1.32	1.27
3	F	349	ITR	CA-N	2.09	1.32	1.27
3	B	349	ITR	CA-N	2.09	1.32	1.27
3	A	349	ITR	CA-N	2.08	1.32	1.27
3	H	349	ITR	CA-N	2.07	1.32	1.27
2	D	348	FAD	C8A-N7A	-2.02	1.31	1.34
2	F	348	FAD	C8A-N7A	-2.02	1.31	1.34

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	348	FAD	C4-N3-C2	11.18	124.58	115.14
2	C	348	FAD	C4-N3-C2	11.12	124.53	115.14
2	E	348	FAD	C4-N3-C2	11.12	124.53	115.14
2	A	348	FAD	C4-N3-C2	11.11	124.52	115.14
2	B	348	FAD	C4-N3-C2	11.11	124.52	115.14
2	H	348	FAD	C4-N3-C2	11.11	124.52	115.14
2	F	348	FAD	C4-N3-C2	11.09	124.51	115.14
2	G	348	FAD	C4-N3-C2	11.09	124.50	115.14
2	G	348	FAD	C1'-N10-C9A	6.86	123.69	118.29
2	B	348	FAD	C1'-N10-C9A	6.86	123.69	118.29
2	D	348	FAD	C1'-N10-C9A	6.85	123.68	118.29
2	E	348	FAD	C1'-N10-C9A	6.83	123.67	118.29
2	A	348	FAD	C1'-N10-C9A	6.83	123.67	118.29
2	H	348	FAD	C1'-N10-C9A	6.82	123.66	118.29
2	F	348	FAD	C1'-N10-C9A	6.81	123.66	118.29
2	C	348	FAD	C1'-N10-C9A	6.76	123.61	118.29
2	D	348	FAD	C4X-C4-N3	-5.22	116.29	123.43
2	C	348	FAD	C4X-C4-N3	-5.22	116.29	123.43
2	E	348	FAD	C4X-C4-N3	-5.20	116.33	123.43
2	A	348	FAD	C4X-C4-N3	-5.19	116.33	123.43
2	H	348	FAD	C4X-C4-N3	-5.19	116.33	123.43
2	B	348	FAD	C4X-C4-N3	-5.18	116.34	123.43
2	F	348	FAD	C4X-C4-N3	-5.18	116.35	123.43
2	G	348	FAD	C4X-C4-N3	-5.15	116.39	123.43
2	C	348	FAD	C10-C4X-N5	5.15	124.82	121.26
2	D	348	FAD	C10-C4X-N5	5.12	124.80	121.26
2	F	348	FAD	C10-C4X-N5	5.10	124.79	121.26
2	B	348	FAD	C10-C4X-N5	5.10	124.78	121.26
2	E	348	FAD	C10-C4X-N5	5.10	124.78	121.26
2	A	348	FAD	C10-C4X-N5	5.10	124.78	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	348	FAD	C5X-C9A-N10	5.08	121.40	117.72
2	H	348	FAD	C10-C4X-N5	5.08	124.77	121.26
2	A	348	FAD	C5X-C9A-N10	5.05	121.37	117.72
2	G	348	FAD	C10-C4X-N5	5.04	124.75	121.26
2	H	348	FAD	C5X-C9A-N10	5.03	121.36	117.72
2	G	348	FAD	C5X-C9A-N10	5.01	121.35	117.72
2	D	348	FAD	C5X-C9A-N10	5.01	121.35	117.72
2	B	348	FAD	C5X-C9A-N10	5.01	121.34	117.72
2	F	348	FAD	C5X-C9A-N10	5.00	121.34	117.72
2	C	348	FAD	C5X-C9A-N10	4.99	121.33	117.72
2	G	348	FAD	C4-C4X-C10	-4.23	117.15	119.95
2	B	348	FAD	C4-C4X-C10	-4.20	117.17	119.95
2	F	348	FAD	C4-C4X-C10	-4.20	117.17	119.95
2	C	348	FAD	C4-C4X-C10	-4.18	117.19	119.95
2	H	348	FAD	C4-C4X-C10	-4.16	117.19	119.95
2	D	348	FAD	C4-C4X-C10	-4.16	117.20	119.95
2	E	348	FAD	C4-C4X-C10	-4.16	117.20	119.95
2	A	348	FAD	C4-C4X-C10	-4.14	117.21	119.95
2	D	348	FAD	C3B-C2B-C1B	-3.33	95.96	100.98
2	A	348	FAD	C3B-C2B-C1B	-3.32	95.99	100.98
2	G	348	FAD	C3B-C2B-C1B	-3.31	95.99	100.98
2	H	348	FAD	C3B-C2B-C1B	-3.31	95.99	100.98
2	F	348	FAD	C3B-C2B-C1B	-3.31	95.99	100.98
2	E	348	FAD	C3B-C2B-C1B	-3.31	95.99	100.98
2	B	348	FAD	C3B-C2B-C1B	-3.31	96.00	100.98
2	C	348	FAD	C3B-C2B-C1B	-3.30	96.01	100.98
2	A	348	FAD	O2B-C2B-C3B	-3.11	101.78	111.82
2	B	348	FAD	O2B-C2B-C3B	-3.10	101.78	111.82
2	D	348	FAD	O2B-C2B-C3B	-3.10	101.78	111.82
2	G	348	FAD	O2B-C2B-C3B	-3.10	101.79	111.82
2	E	348	FAD	O2B-C2B-C3B	-3.10	101.79	111.82
2	F	348	FAD	O2B-C2B-C3B	-3.10	101.81	111.82
2	H	348	FAD	O2B-C2B-C3B	-3.09	101.83	111.82
2	C	348	FAD	O2B-C2B-C3B	-3.09	101.83	111.82
2	G	348	FAD	C4X-C10-N10	-2.90	117.32	120.30
2	H	348	FAD	C4X-C10-N10	-2.90	117.32	120.30
2	C	348	FAD	C4X-C10-N10	-2.90	117.33	120.30
2	F	348	FAD	P-O3P-PA	-2.89	122.91	132.83
2	A	348	FAD	P-O3P-PA	-2.89	122.91	132.83
2	B	348	FAD	P-O3P-PA	-2.89	122.92	132.83
2	D	348	FAD	C4X-C10-N10	-2.89	117.34	120.30
2	E	348	FAD	P-O3P-PA	-2.88	122.93	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	348	FAD	P-O3P-PA	-2.88	122.94	132.83
2	H	348	FAD	P-O3P-PA	-2.88	122.95	132.83
2	G	348	FAD	P-O3P-PA	-2.88	122.96	132.83
2	D	348	FAD	P-O3P-PA	-2.88	122.96	132.83
2	E	348	FAD	C4X-C10-N10	-2.86	117.36	120.30
2	A	348	FAD	C4X-C10-N10	-2.85	117.38	120.30
2	F	348	FAD	C4X-C10-N10	-2.84	117.38	120.30
2	B	348	FAD	C4X-C10-N10	-2.83	117.39	120.30
2	F	348	FAD	C9A-N10-C10	-2.63	118.46	121.91
2	B	348	FAD	C9A-N10-C10	-2.63	118.47	121.91
2	A	348	FAD	C9A-N10-C10	-2.61	118.48	121.91
2	E	348	FAD	C9A-N10-C10	-2.60	118.50	121.91
2	D	348	FAD	C9A-N10-C10	-2.59	118.52	121.91
2	G	348	FAD	C9A-N10-C10	-2.58	118.53	121.91
2	C	348	FAD	C9A-N10-C10	-2.58	118.53	121.91
2	H	348	FAD	C9A-N10-C10	-2.57	118.55	121.91
3	C	349	ITR	CG-CB-CA	-2.45	107.77	113.62
3	H	349	ITR	CG-CB-CA	-2.45	107.79	113.62
3	E	349	ITR	CG-CB-CA	-2.44	107.80	113.62
3	D	349	ITR	CG-CB-CA	-2.44	107.80	113.62
3	B	349	ITR	CG-CB-CA	-2.44	107.81	113.62
3	G	349	ITR	CG-CB-CA	-2.43	107.81	113.62
3	A	349	ITR	CG-CB-CA	-2.43	107.82	113.62
3	F	349	ITR	CG-CB-CA	-2.43	107.83	113.62
2	H	348	FAD	C7M-C7-C8	-2.34	115.94	120.74
2	E	348	FAD	C7M-C7-C8	-2.33	115.96	120.74
2	A	348	FAD	C7M-C7-C8	-2.33	115.97	120.74
2	B	348	FAD	C7M-C7-C8	-2.32	115.97	120.74
2	F	348	FAD	C7M-C7-C8	-2.32	115.98	120.74
2	D	348	FAD	C7M-C7-C8	-2.32	115.98	120.74
2	B	348	FAD	C4'-C3'-C2'	-2.32	108.53	113.36
2	C	348	FAD	C7M-C7-C8	-2.32	115.98	120.74
2	G	348	FAD	C4'-C3'-C2'	-2.30	108.57	113.36
2	D	348	FAD	C4'-C3'-C2'	-2.30	108.59	113.36
2	A	348	FAD	C4'-C3'-C2'	-2.29	108.59	113.36
2	G	348	FAD	C7M-C7-C8	-2.29	116.03	120.74
2	E	348	FAD	C4'-C3'-C2'	-2.29	108.59	113.36
2	H	348	FAD	C4'-C3'-C2'	-2.29	108.60	113.36
2	C	348	FAD	C4'-C3'-C2'	-2.28	108.63	113.36
2	F	348	FAD	C4'-C3'-C2'	-2.27	108.63	113.36

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	348	FAD	C5B-O5B-PA-O2A
2	E	348	FAD	C5B-O5B-PA-O2A
2	B	348	FAD	C5B-O5B-PA-O2A
2	F	348	FAD	C5B-O5B-PA-O2A
2	D	348	FAD	C5B-O5B-PA-O2A
2	H	348	FAD	C5B-O5B-PA-O2A
2	C	348	FAD	C5B-O5B-PA-O2A
2	A	348	FAD	C5B-O5B-PA-O2A
2	G	348	FAD	O4B-C4B-C5B-O5B
2	G	348	FAD	C3B-C4B-C5B-O5B
2	E	348	FAD	O4B-C4B-C5B-O5B
2	E	348	FAD	C3B-C4B-C5B-O5B
2	B	348	FAD	O4B-C4B-C5B-O5B
2	B	348	FAD	C3B-C4B-C5B-O5B
2	F	348	FAD	O4B-C4B-C5B-O5B
2	F	348	FAD	C3B-C4B-C5B-O5B
2	D	348	FAD	O4B-C4B-C5B-O5B
2	D	348	FAD	C3B-C4B-C5B-O5B
2	H	348	FAD	O4B-C4B-C5B-O5B
2	H	348	FAD	C3B-C4B-C5B-O5B
2	C	348	FAD	O4B-C4B-C5B-O5B
2	C	348	FAD	C3B-C4B-C5B-O5B
2	A	348	FAD	O4B-C4B-C5B-O5B
2	A	348	FAD	C3B-C4B-C5B-O5B
2	G	348	FAD	C5B-O5B-PA-O3P
2	E	348	FAD	C5B-O5B-PA-O3P
2	B	348	FAD	C5B-O5B-PA-O3P
2	F	348	FAD	C5B-O5B-PA-O3P
2	D	348	FAD	C5B-O5B-PA-O3P
2	H	348	FAD	C5B-O5B-PA-O3P
2	C	348	FAD	C5B-O5B-PA-O3P
2	A	348	FAD	C5B-O5B-PA-O3P
2	G	348	FAD	C5B-O5B-PA-O1A
2	E	348	FAD	C5B-O5B-PA-O1A
2	B	348	FAD	C5B-O5B-PA-O1A
2	F	348	FAD	C5B-O5B-PA-O1A
2	D	348	FAD	C5B-O5B-PA-O1A
2	H	348	FAD	C5B-O5B-PA-O1A
2	C	348	FAD	C5B-O5B-PA-O1A
2	A	348	FAD	C5B-O5B-PA-O1A

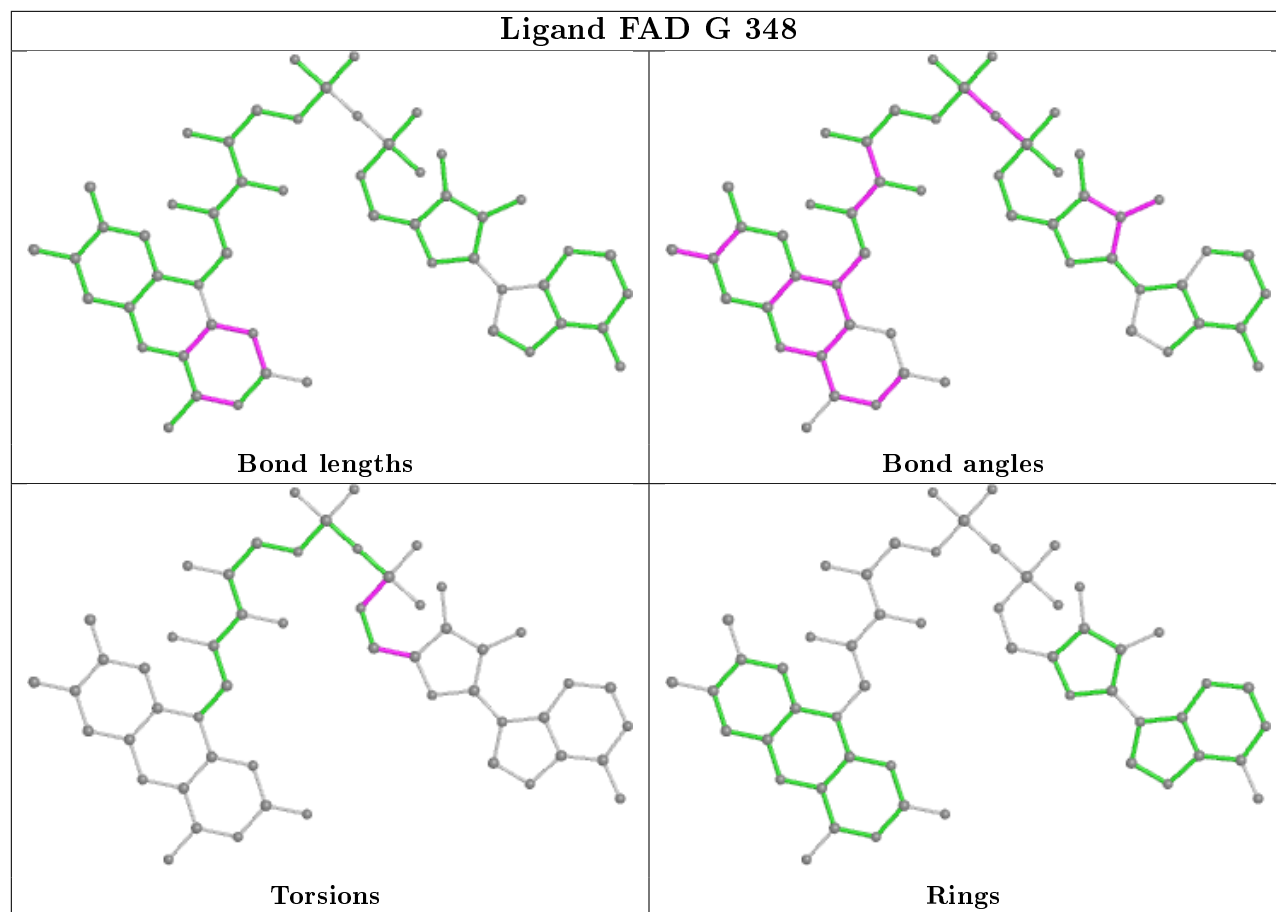
There are no ring outliers.

9 monomers are involved in 33 short contacts:

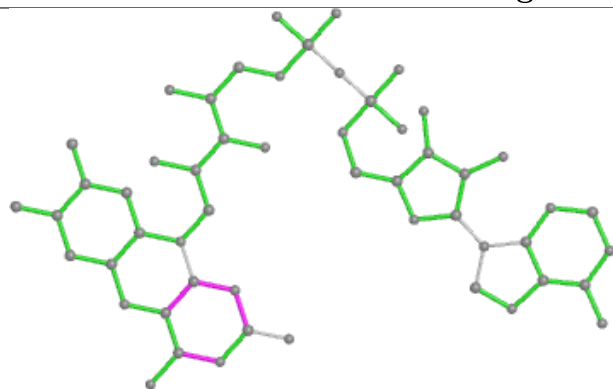
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	348	FAD	5	0
2	E	348	FAD	2	0
2	A	348	FAD	5	0
2	B	348	FAD	3	0
2	F	348	FAD	4	0
2	D	348	FAD	4	0
3	F	349	ITR	1	0
2	H	348	FAD	5	0
2	C	348	FAD	4	0

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.

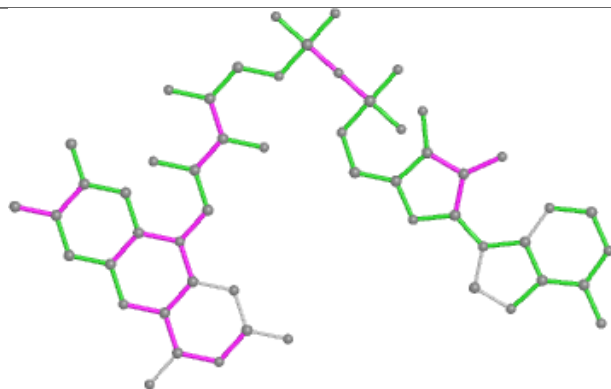




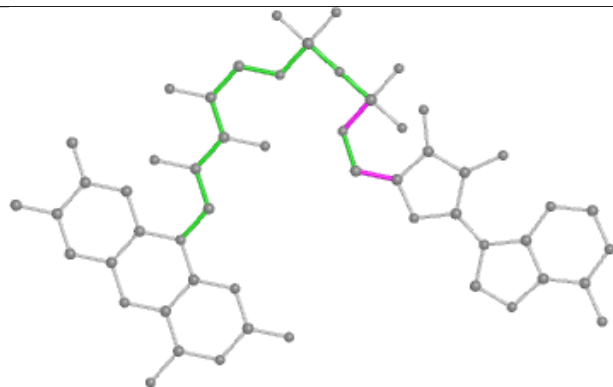
## Ligand FAD E 348



Bond lengths



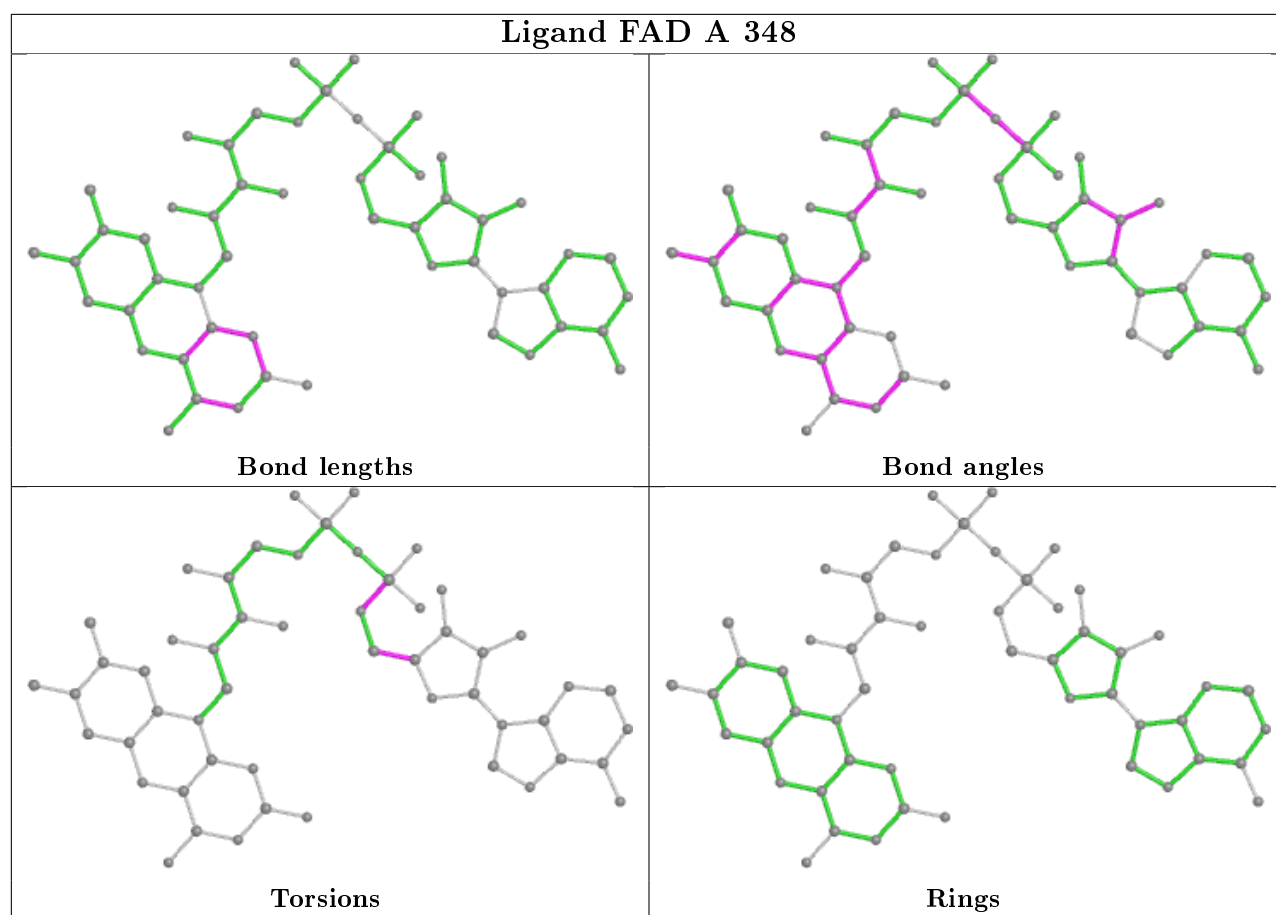
Bond angles



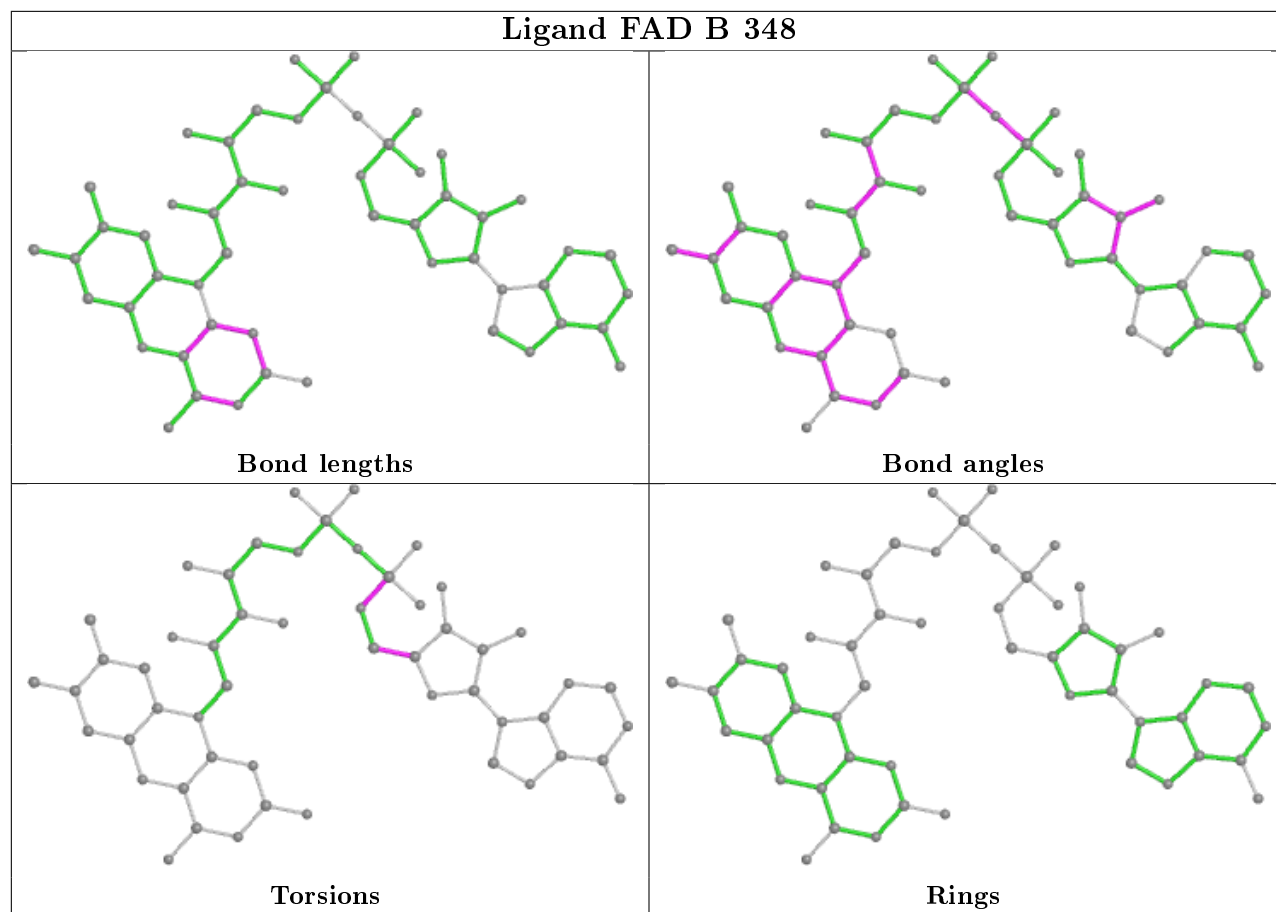
Torsions



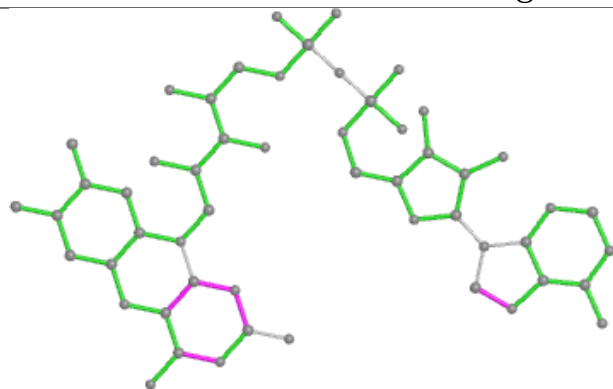
Rings



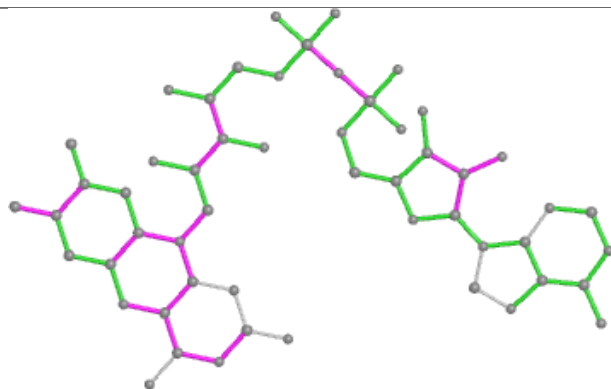
## Ligand FAD B 348



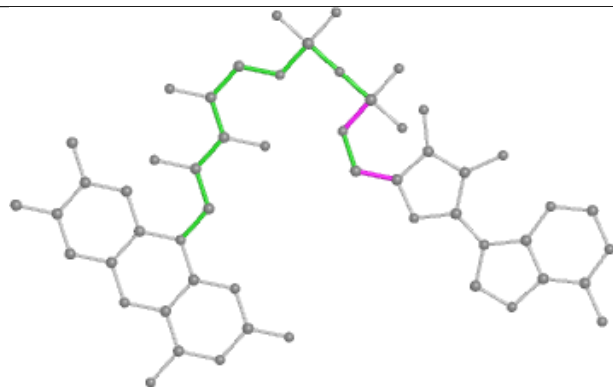
## Ligand FAD F 348



Bond lengths



Bond angles

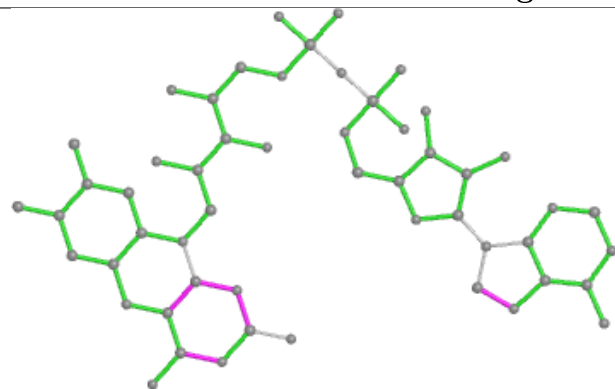


Torsions

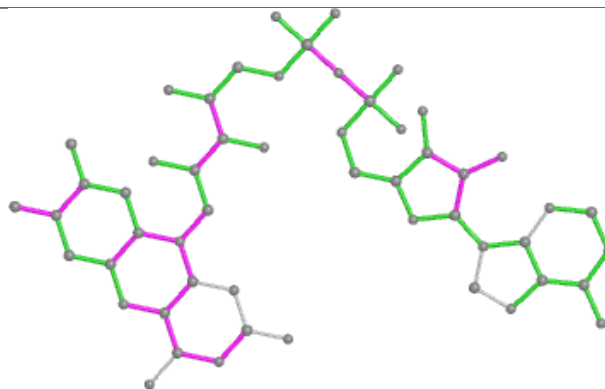


Rings

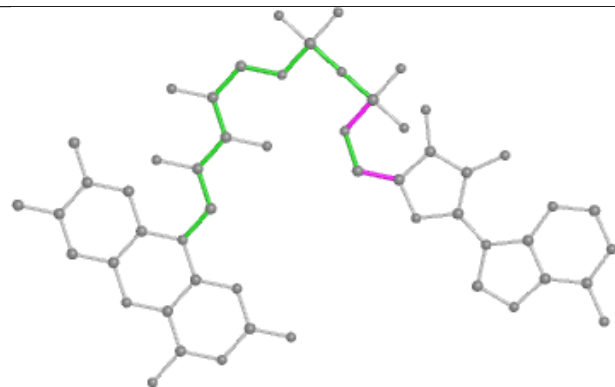
## Ligand FAD D 348



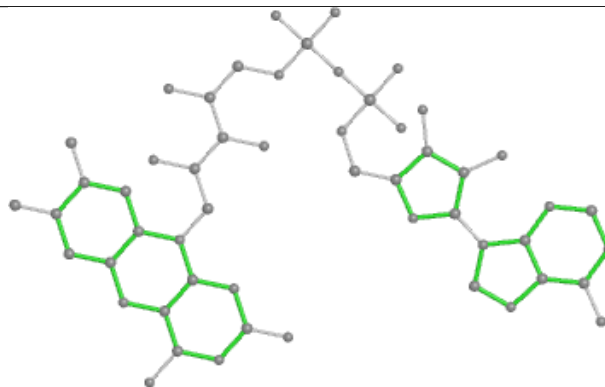
Bond lengths



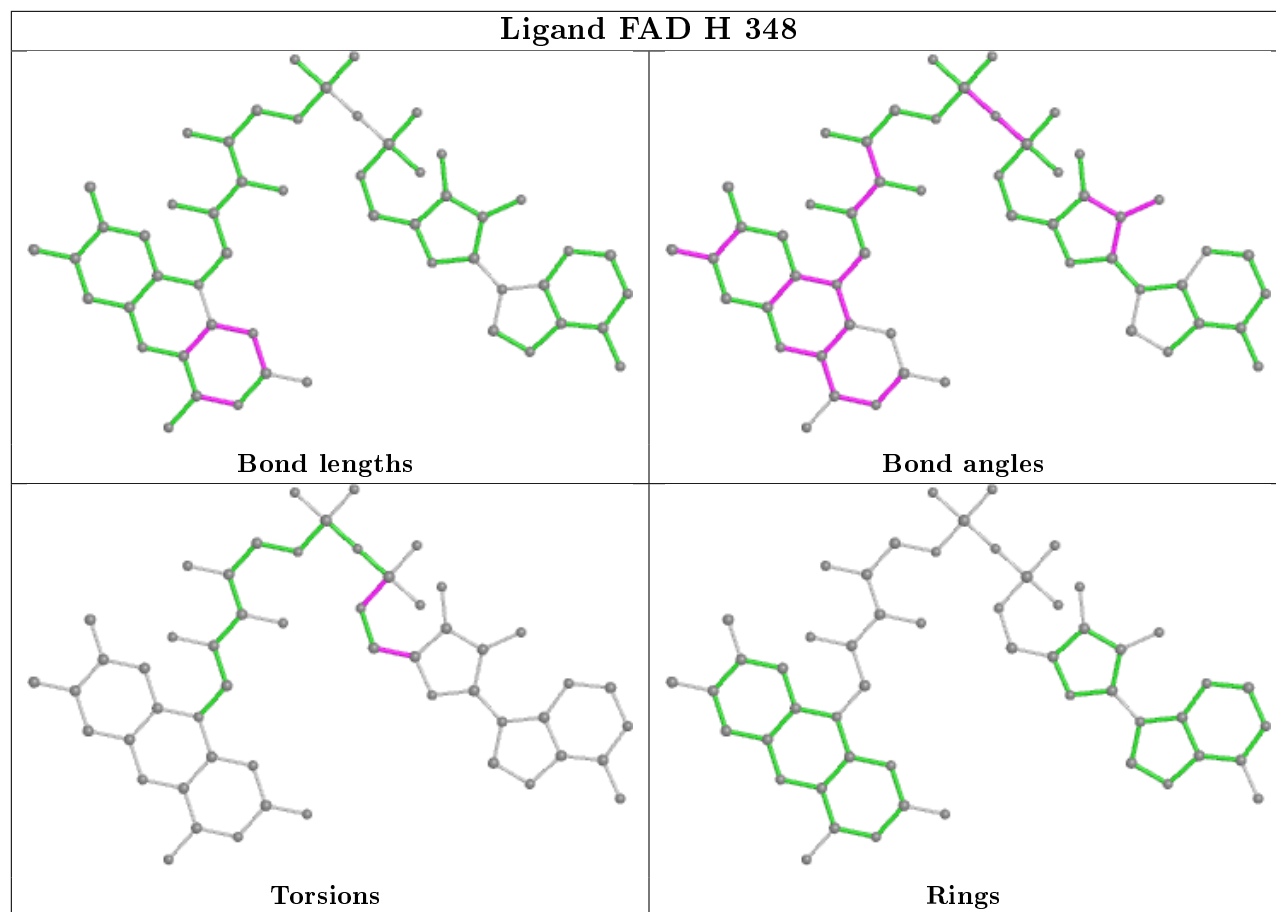
Bond angles

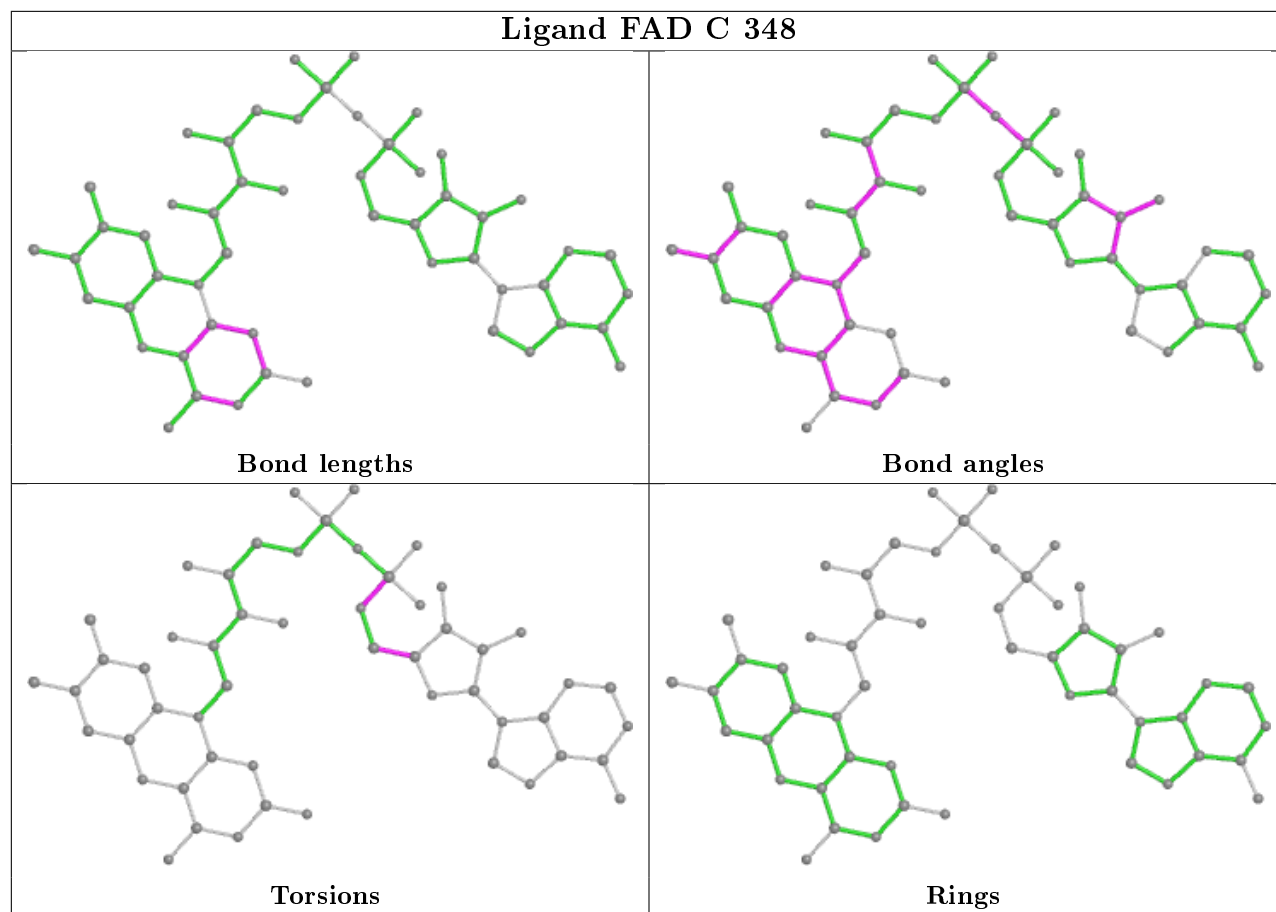


Torsions



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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	330/347 (95%)	0.07	6 (1%) 68 47	18, 35, 71, 100	23 (6%)
1	B	328/347 (94%)	0.44	35 (10%) 6 2	18, 36, 77, 100	24 (7%)
1	C	331/347 (95%)	0.11	13 (3%) 39 20	18, 36, 82, 100	26 (7%)
1	D	332/347 (95%)	0.18	8 (2%) 59 37	12, 36, 69, 100	19 (5%)
1	E	331/347 (95%)	0.32	18 (5%) 25 12	18, 36, 78, 100	26 (7%)
1	F	329/347 (94%)	0.01	6 (1%) 68 47	18, 36, 70, 100	19 (5%)
1	G	327/347 (94%)	0.90	43 (13%) 3 1	18, 36, 83, 100	26 (7%)
1	H	329/347 (94%)	0.18	8 (2%) 59 37	18, 36, 73, 100	22 (6%)
All	All	2637/2776 (94%)	0.28	137 (5%) 27 12	12, 36, 76, 100	185 (7%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	301	SER	12.5
1	G	300	SER	7.4
1	D	299	GLY	6.4
1	G	299	GLY	5.8
1	D	301	SER	5.7
1	B	300	SER	5.2
1	B	299	GLY	4.8
1	D	300	SER	4.8
1	B	303	THR	4.6
1	G	327	ALA	4.3
1	G	298	PHE	4.2
1	B	334	LEU	4.1
1	C	24	HIS	4.1
1	F	123	ASP	3.9
1	G	307	HIS	3.8
1	H	298	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	335	GLU	3.7
1	G	305	VAL	3.7
1	B	31	ASP	3.6
1	B	62	PRO	3.5
1	C	298	PHE	3.5
1	G	181	CYS	3.5
1	F	300	SER	3.4
1	G	175	ALA	3.3
1	G	336	GLU	3.3
1	E	71	THR	3.3
1	A	123	ASP	3.3
1	G	303	THR	3.3
1	E	26	VAL	3.3
1	G	7	GLY	3.2
1	E	24	HIS	3.2
1	H	335	GLU	3.1
1	G	71	THR	3.1
1	G	191	PRO	3.1
1	B	160	PHE	3.1
1	B	21	GLU	3.1
1	A	301	SER	3.0
1	A	160	PHE	3.0
1	G	67	TRP	3.0
1	D	24	HIS	3.0
1	C	335	GLU	2.9
1	B	18	CYS	2.9
1	B	66	ASN	2.9
1	G	224	TYR	2.9
1	B	336	GLU	2.9
1	C	303	THR	2.9
1	E	67	TRP	2.9
1	G	31	ASP	2.9
1	C	327	ALA	2.9
1	F	301	SER	2.8
1	B	333	VAL	2.8
1	B	331	GLY	2.8
1	G	68	ASN	2.8
1	B	175	ALA	2.8
1	B	335	GLU	2.7
1	E	335	GLU	2.7
1	H	24	HIS	2.7
1	B	337	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	299	GLY	2.7
1	B	3	VAL	2.7
1	E	66	ASN	2.7
1	E	333	VAL	2.7
1	B	67	TRP	2.6
1	B	24	HIS	2.6
1	H	307	HIS	2.6
1	E	123	ASP	2.6
1	G	246	ASN	2.6
1	B	70	GLN	2.6
1	H	301	SER	2.6
1	C	67	TRP	2.5
1	G	285	VAL	2.5
1	B	298	PHE	2.5
1	B	57	SER	2.5
1	B	68	ASN	2.5
1	G	297	ARG	2.5
1	B	156	GLY	2.5
1	C	175	ALA	2.5
1	D	224	TYR	2.5
1	A	25	SER	2.5
1	B	307	HIS	2.4
1	E	2	ARG	2.4
1	G	194	LEU	2.4
1	G	294	GLU	2.4
1	B	177	VAL	2.4
1	E	59	PRO	2.4
1	A	300	SER	2.4
1	C	323	ALA	2.4
1	G	177	VAL	2.4
1	A	337	ARG	2.4
1	B	71	THR	2.4
1	C	299	GLY	2.4
1	G	292	GLU	2.4
1	G	59	PRO	2.3
1	G	242	PHE	2.3
1	B	171	ALA	2.3
1	E	31	ASP	2.3
1	G	287	PRO	2.3
1	B	20	HIS	2.3
1	G	219	LEU	2.3
1	G	169	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	328	LYS	2.3
1	D	298	PHE	2.3
1	E	22	ARG	2.3
1	D	303	THR	2.3
1	G	313	GLY	2.3
1	B	329	LEU	2.3
1	G	218	ASP	2.3
1	G	176	ASP	2.2
1	G	304	GLU	2.2
1	G	192	ASP	2.2
1	G	66	ASN	2.2
1	H	221	ARG	2.2
1	B	2	ARG	2.2
1	G	70	GLN	2.2
1	B	306	ILE	2.2
1	E	68	ASN	2.2
1	C	191	PRO	2.2
1	E	57	SER	2.2
1	C	70	GLN	2.2
1	C	71	THR	2.2
1	G	174	GLY	2.1
1	G	334	LEU	2.1
1	E	94	GLY	2.1
1	G	264	CYS	2.1
1	H	292	GLU	2.1
1	F	224	TYR	2.1
1	B	294	GLU	2.1
1	B	69	GLN	2.1
1	G	160	PHE	2.1
1	B	324	LEU	2.1
1	E	323	ALA	2.1
1	D	57	SER	2.1
1	E	23	TYR	2.0
1	H	321	GLY	2.0
1	G	195	LEU	2.0
1	F	299	GLY	2.0
1	F	335	GLU	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 ⓘ

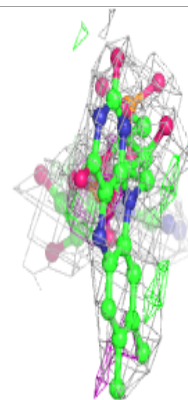
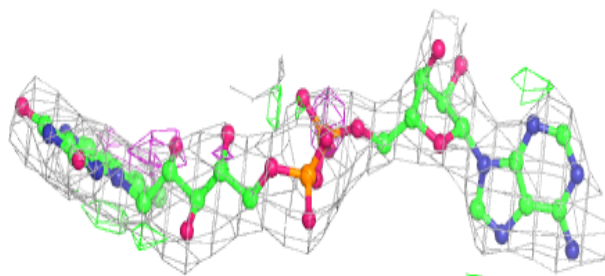
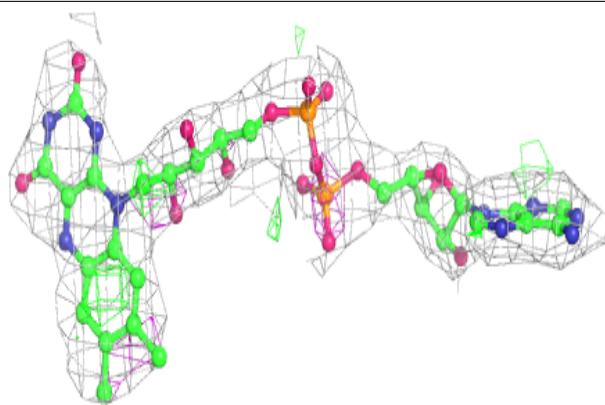
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	ITR	H	349	15/15	0.85	0.31	45,52,58,72	0
3	ITR	E	349	15/15	0.85	0.31	45,52,58,72	0
3	ITR	C	349	15/15	0.86	0.33	45,52,58,72	0
3	ITR	F	349	15/15	0.88	0.29	45,52,58,72	0
3	ITR	D	349	15/15	0.88	0.30	45,52,58,72	0
3	ITR	G	349	15/15	0.89	0.34	45,52,58,72	0
4	DTR	E	350	15/15	0.90	0.37	9,42,100,100	0
4	DTR	F	350	15/15	0.91	0.40	1,49,100,100	0
2	FAD	G	348	53/53	0.94	0.37	20,27,42,43	0
3	ITR	A	349	15/15	0.94	0.28	45,52,58,72	0
2	FAD	B	348	53/53	0.94	0.27	20,27,42,43	0
3	ITR	B	349	15/15	0.94	0.27	45,52,58,72	0
2	FAD	A	348	53/53	0.94	0.25	20,27,42,43	0
2	FAD	D	348	53/53	0.94	0.27	20,27,42,43	0
2	FAD	C	348	53/53	0.95	0.26	20,27,42,43	0
2	FAD	E	348	53/53	0.95	0.24	20,27,42,43	0
2	FAD	H	348	53/53	0.96	0.26	20,27,42,43	0
2	FAD	F	348	53/53	0.96	0.24	20,27,42,43	0

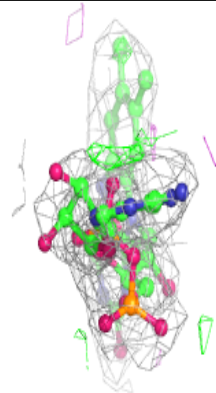
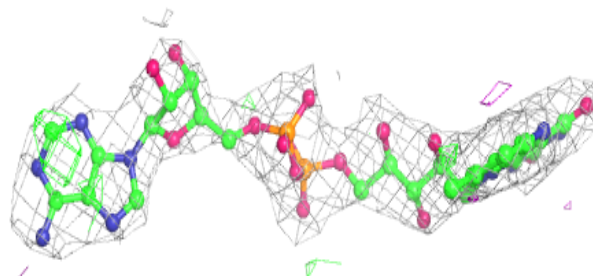
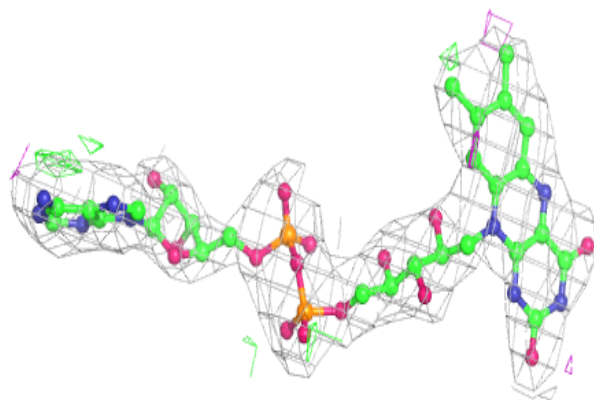
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around FAD G 348:**

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

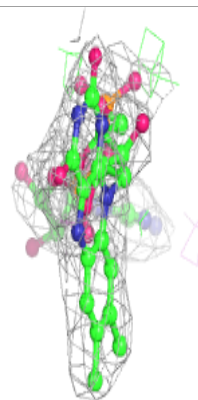
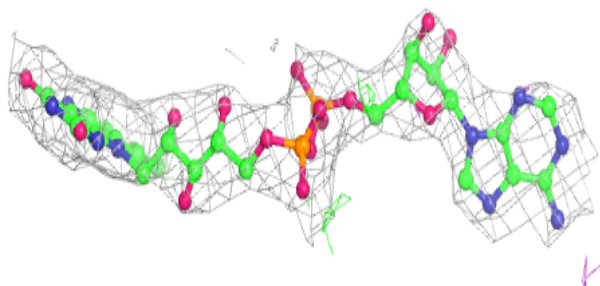
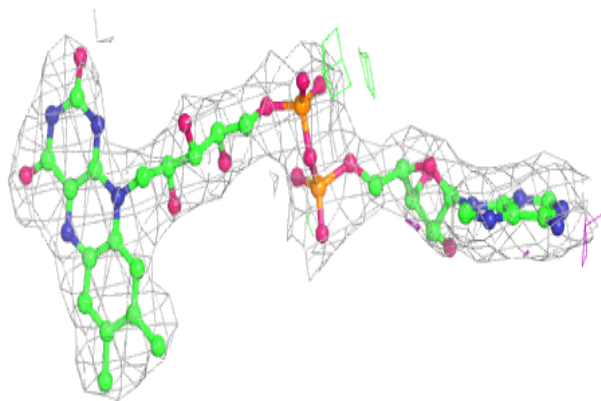
**Electron density around FAD B 348:**

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

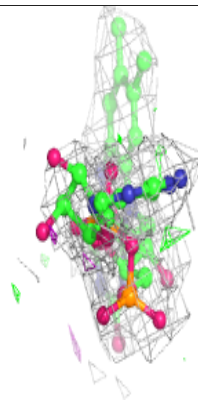
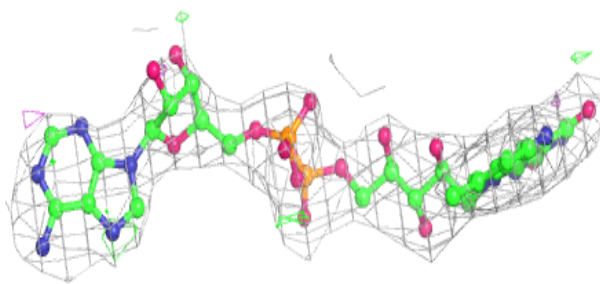
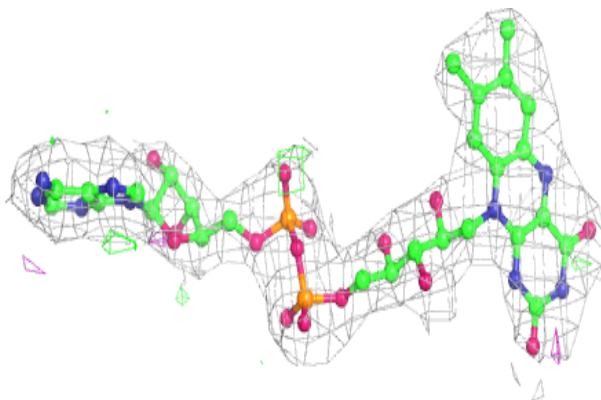


**Electron density around FAD A 348:**

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

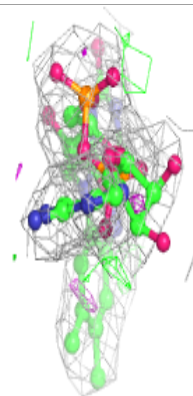
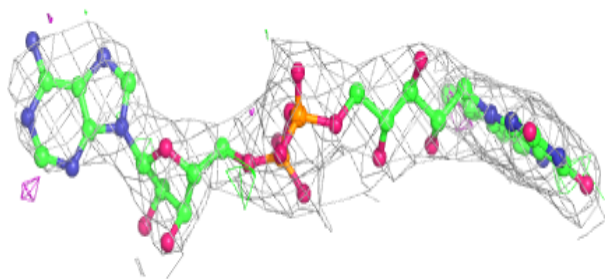
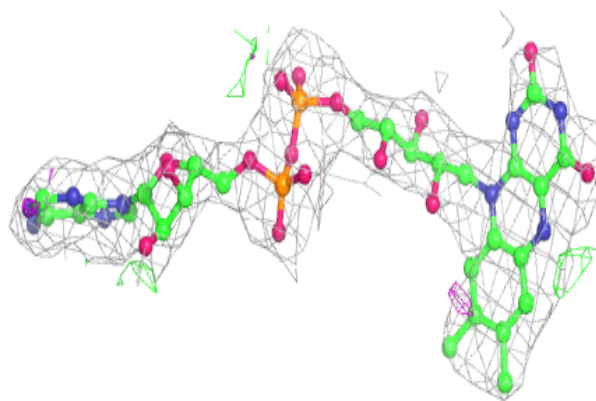
**Electron density around FAD D 348:**

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

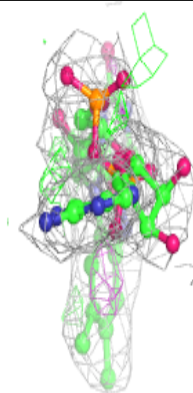
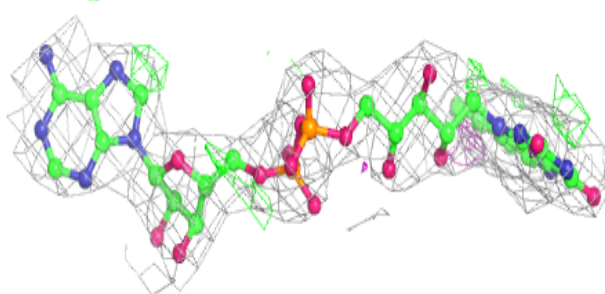
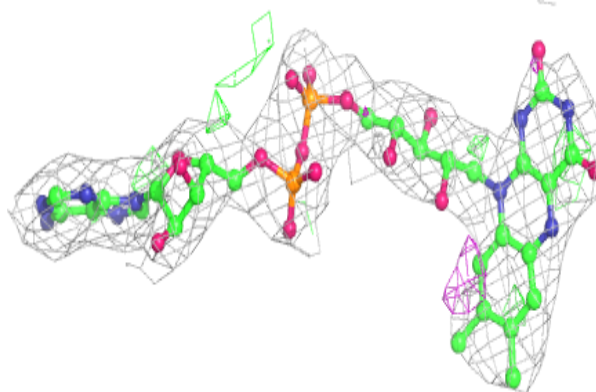


**Electron density around FAD C 348:**

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

**Electron density around FAD E 348:**

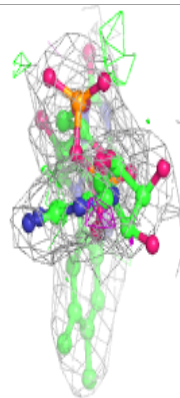
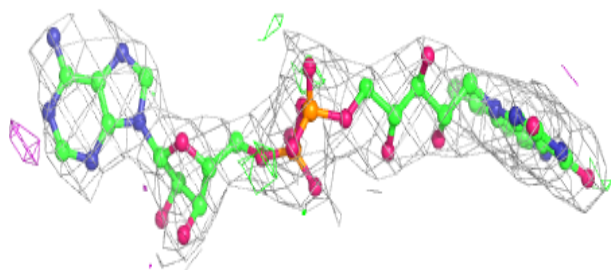
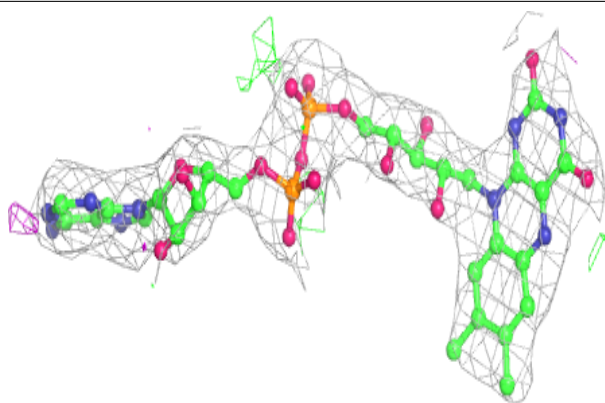
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



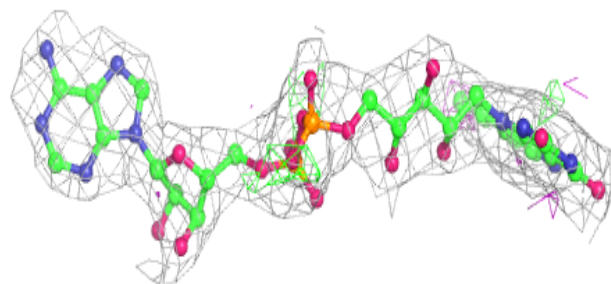
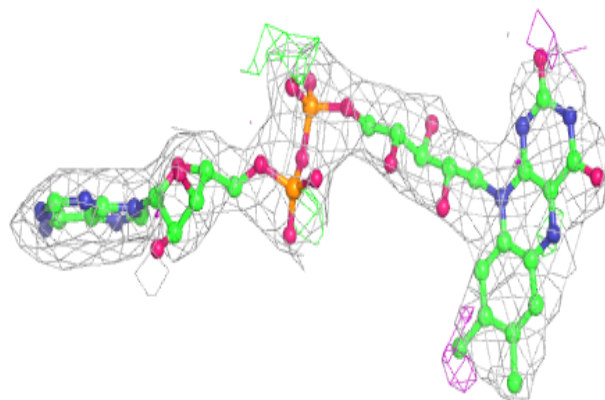


**Electron density around FAD H 348:**

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

**Electron density around FAD F 348:**

$2mF_o-DF_c$  (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.