



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 1EGE / pdb_00001ege
Title : STRUCTURE OF T255E, E376G MUTANT OF HUMAN MEDIUM CHAIN
ACYL-COA DEHYDROGENASE
Authors : Lee, H.J.; Wang, M.; Paschke, R.; Nandy, A.; Ghisla, S.; Kim, J.P.
Deposited on : 1996-04-11
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

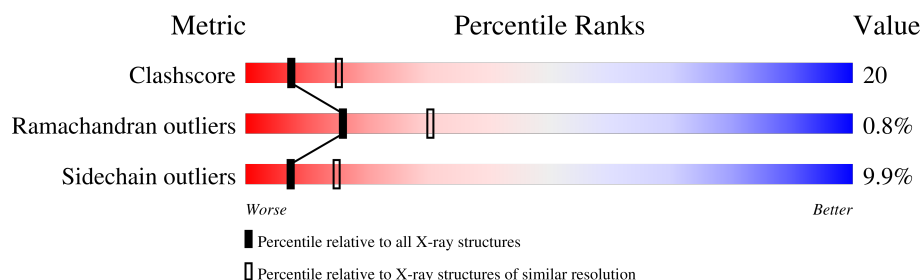
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	
1	B	396	
1	C	396	
1	D	396	

2 Entry composition [i](#)

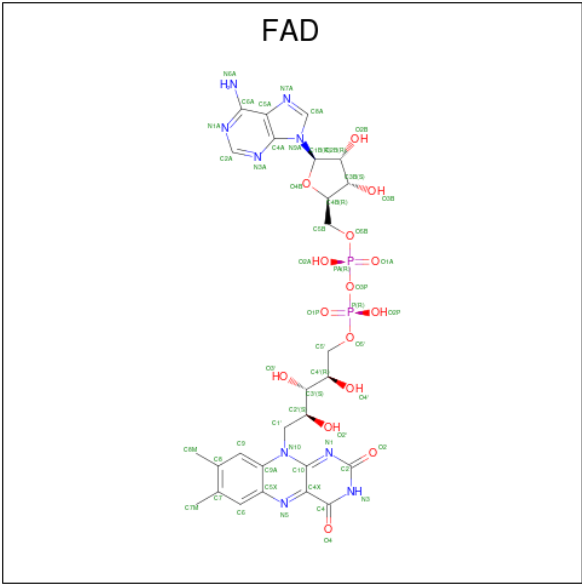
There are 2 unique types of molecules in this entry. The entry contains 12184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MEDIUM CHAIN ACYL-COA DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2993	1894	515	566	18			
1	B	387	Total	C	N	O	S	0	0	0
			2993	1894	515	566	18			
1	C	387	Total	C	N	O	S	0	0	0
			2993	1894	515	566	18			
1	D	387	Total	C	N	O	S	0	0	0
			2993	1894	515	566	18			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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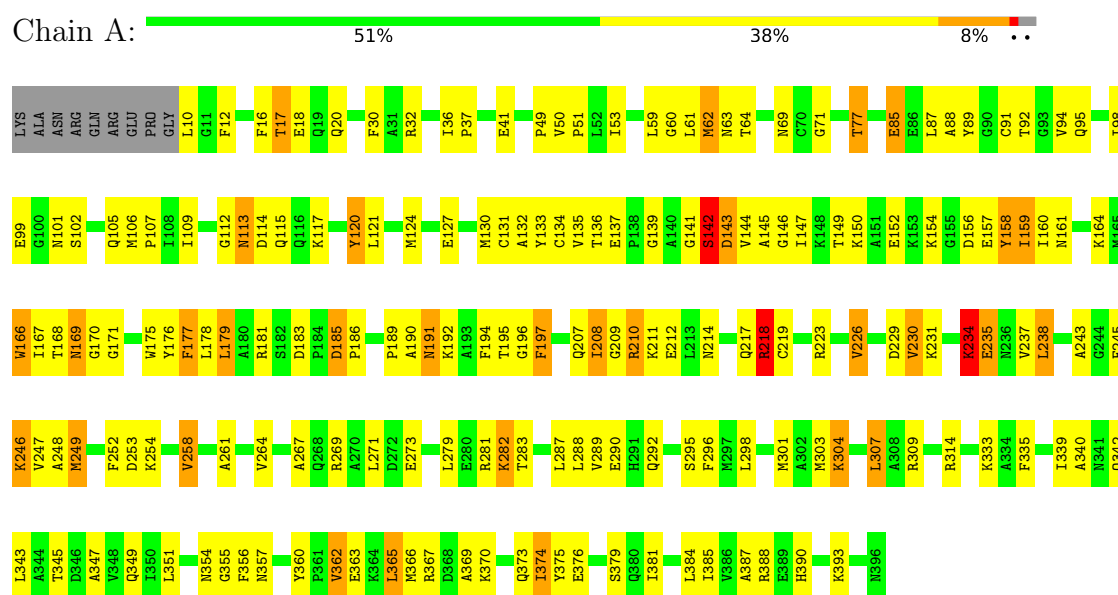
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

3 Residue-property plots

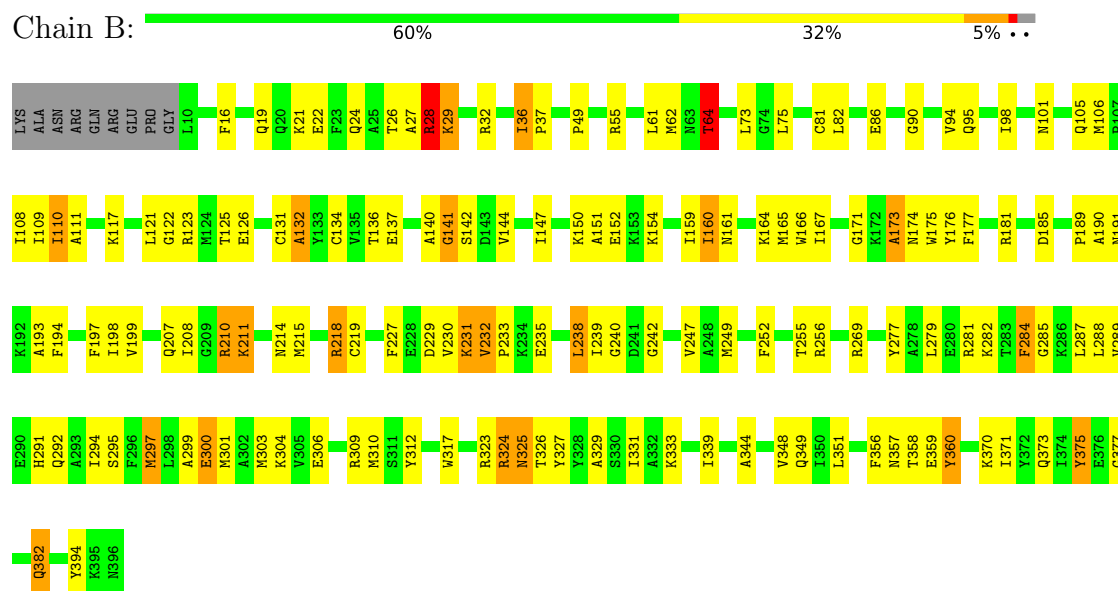
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

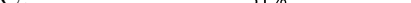
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

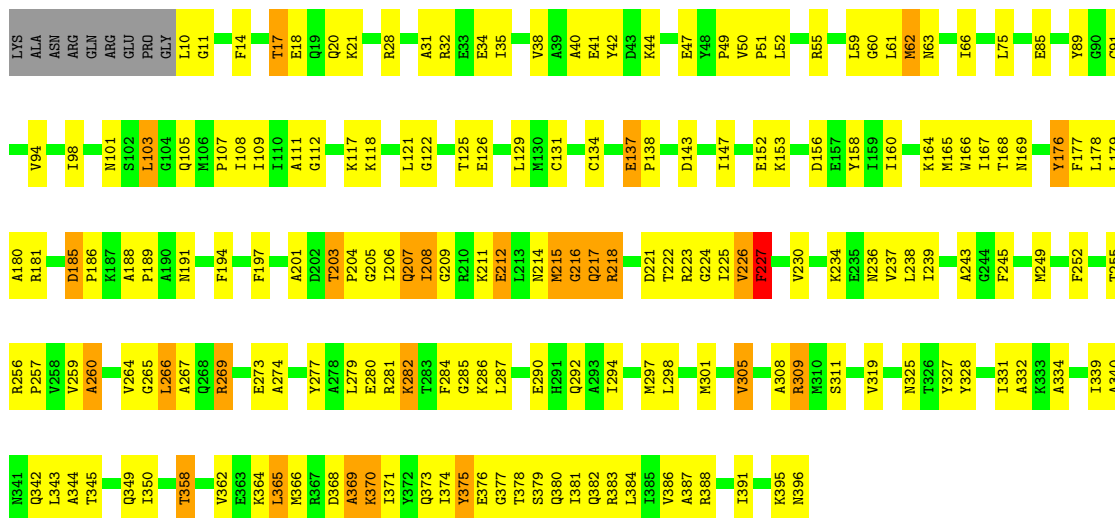


• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

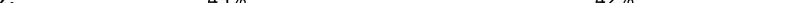


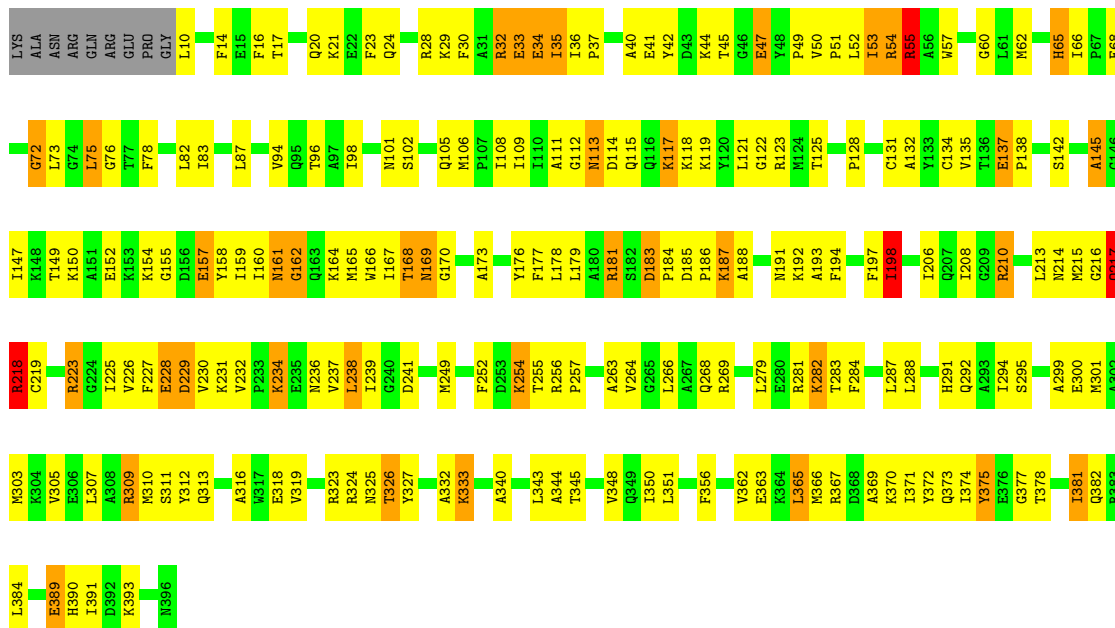
- Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C:  51% 40% 7%



- Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D:  45% 42% 9% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.59Å 169.59Å 151.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.75	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.75)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.221 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12184	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.63	3/3048 (0.1%)	1.21	25/4107 (0.6%)
1	B	1.21	4/3048 (0.1%)	1.80	27/4107 (0.7%)
1	C	0.78	10/3048 (0.3%)	1.15	30/4107 (0.7%)
1	D	0.89	18/3048 (0.6%)	1.18	24/4107 (0.6%)
All	All	0.90	35/12192 (0.3%)	1.36	106/16428 (0.6%)

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	3
1	B	0	2
1	C	0	3
1	D	0	8
All	All	0	16

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	PHE	CD2-CE2	46.84	2.79	1.38
1	B	324	ARG	C-N	-27.39	1.00	1.33
1	C	284	PHE	CG-CD1	16.52	1.73	1.38
1	D	214	ASN	C-N	-12.77	1.14	1.33
1	C	284	PHE	CG-CD2	-11.92	1.13	1.38
1	C	60	GLY	C-N	11.06	1.51	1.33
1	D	32	ARG	C-N	10.14	1.47	1.33
1	D	113	ASN	C-N	-8.91	1.23	1.33
1	C	226	VAL	C-N	-8.90	1.18	1.33
1	A	214	ASN	C-N	-8.65	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	ASN	CG-ND2	-7.98	1.16	1.33
1	D	60	GLY	C-N	-7.46	1.24	1.33
1	D	76	GLY	N-CA	6.97	1.54	1.45
1	C	214	ASN	C-N	-6.62	1.24	1.33
1	D	217	GLN	C-N	6.46	1.42	1.33
1	C	206	ILE	C-N	-6.41	1.24	1.33
1	D	34	GLU	N-CA	6.29	1.54	1.46
1	D	162	GLY	C-N	6.09	1.41	1.33
1	C	285	GLY	C-N	5.93	1.40	1.33
1	C	281	ARG	C-N	-5.92	1.25	1.33
1	D	47	GLU	C-N	5.92	1.41	1.33
1	D	161	ASN	C-N	5.91	1.39	1.33
1	D	229	ASP	C-N	5.72	1.40	1.33
1	A	60	GLY	C-N	-5.68	1.26	1.33
1	D	34	GLU	CA-C	5.57	1.58	1.53
1	B	323	ARG	C-N	5.47	1.41	1.33
1	C	189	PRO	C-N	-5.41	1.26	1.33
1	D	35	ILE	N-CA	5.38	1.53	1.46
1	D	33	GLU	CA-C	5.34	1.59	1.52
1	D	162	GLY	CA-C	5.30	1.57	1.51
1	B	21	LYS	C-N	5.27	1.41	1.33
1	A	226	VAL	C-N	-5.20	1.24	1.33
1	D	226	VAL	C-N	-5.16	1.26	1.33
1	C	215	MET	C-N	-5.12	1.28	1.34
1	D	281	ARG	C-N	-5.05	1.26	1.33

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	284	PHE	CE1-CZ-CE2	-65.95	1.28	120.00
1	B	284	PHE	CG-CD2-CE2	-35.90	59.67	120.70
1	B	284	PHE	CZ-CE2-CD2	-33.11	60.40	120.00
1	B	324	ARG	CA-C-N	23.80	152.06	120.65
1	B	324	ARG	C-N-CA	23.80	152.06	120.65
1	A	169	ASN	O-C-N	-23.61	97.08	121.87
1	D	218	ARG	O-C-N	-14.26	107.01	122.12
1	C	284	PHE	CB-CG-CD2	12.89	142.61	120.70
1	A	64	THR	O-C-N	-12.13	108.16	122.11
1	A	218	ARG	O-C-N	-11.57	110.05	122.09
1	C	218	ARG	O-C-N	-10.62	103.22	122.34
1	B	64	THR	O-C-N	-10.18	108.78	122.43
1	C	284	PHE	CB-CG-CD1	-10.09	103.54	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	168	THR	O-C-N	9.41	134.05	123.04
1	D	47	GLU	O-C-N	8.43	133.18	122.81
1	C	226	VAL	CA-C-N	8.17	133.46	122.84
1	C	226	VAL	C-N-CA	8.17	133.46	122.84
1	D	198	ILE	N-CA-C	-7.78	99.58	109.30
1	A	177	PHE	N-CA-C	-7.69	97.15	109.76
1	A	217	GLN	O-C-N	7.63	132.01	122.55
1	C	60	GLY	CA-C-N	-7.52	108.82	122.50
1	C	60	GLY	C-N-CA	-7.52	108.82	122.50
1	D	169	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	D	177	PHE	N-CA-C	-7.38	97.55	109.96
1	A	166	TRP	CA-C-N	-7.02	113.59	122.37
1	A	166	TRP	C-N-CA	-7.02	113.59	122.37
1	A	159	ILE	CA-C-N	-6.95	114.04	123.14
1	A	159	ILE	C-N-CA	-6.95	114.04	123.14
1	B	325	ASN	O-C-N	6.93	129.24	122.03
1	D	65	HIS	O-C-N	-6.83	113.87	122.27
1	D	112	GLY	O-C-N	6.59	131.12	123.21
1	A	230	VAL	O-C-N	6.51	130.13	122.83
1	D	53	ILE	N-CA-C	-6.44	104.24	110.42
1	B	327	TYR	O-C-N	-6.40	115.33	122.12
1	B	177	PHE	N-CA-C	-6.39	99.23	109.96
1	C	236	ASN	O-C-N	-6.33	114.27	122.37
1	B	240	GLY	O-C-N	6.30	132.81	122.42
1	C	281	ARG	O-C-N	-6.26	115.93	123.13
1	A	374	ILE	N-CA-C	6.25	117.36	111.48
1	C	224	GLY	N-CA-C	-6.25	103.02	112.89
1	C	177	PHE	N-CA-C	-6.24	99.07	109.24
1	C	17	THR	N-CA-C	-6.17	101.14	110.28
1	B	21	LYS	CA-C-N	-6.10	110.46	121.14
1	B	21	LYS	C-N-CA	-6.10	110.46	121.14
1	C	255	THR	N-CA-C	6.04	117.94	111.36
1	B	239	ILE	N-CA-C	-6.01	107.43	113.20
1	A	62	MET	O-C-N	5.98	131.13	123.11
1	C	284	PHE	CG-CD2-CE2	5.97	130.84	120.70
1	A	238	LEU	N-CA-C	5.96	119.02	111.69
1	C	205	GLY	O-C-N	-5.93	114.99	122.70
1	A	362	VAL	N-CA-C	5.90	117.35	110.62
1	D	155	GLY	O-C-N	5.88	130.35	122.70
1	D	35	ILE	O-C-N	-5.87	115.24	122.57
1	A	369	ALA	N-CA-C	5.80	118.35	111.33
1	C	238	LEU	N-CA-C	5.80	117.29	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	227	PHE	CA-C-N	5.78	132.80	123.33
1	C	227	PHE	C-N-CA	5.78	132.80	123.33
1	B	331	ILE	N-CA-C	-5.75	104.76	110.62
1	D	183	ASP	CA-C-N	5.74	125.60	119.28
1	D	183	ASP	C-N-CA	5.74	125.60	119.28
1	C	369	ALA	N-CA-C	5.74	117.54	111.28
1	C	362	VAL	N-CA-C	5.62	116.27	110.36
1	B	218	ARG	O-C-N	-5.58	115.84	122.20
1	C	189	PRO	CA-C-N	5.46	131.98	121.54
1	C	189	PRO	C-N-CA	5.46	131.98	121.54
1	B	360	TYR	CA-C-N	5.45	124.97	119.19
1	B	360	TYR	C-N-CA	5.45	124.97	119.19
1	C	370	LYS	N-CA-C	5.45	117.22	111.28
1	B	173	ALA	N-CA-C	5.44	119.09	109.96
1	D	216	GLY	O-C-N	5.41	128.59	123.56
1	D	72	GLY	CA-C-N	5.41	128.07	120.28
1	D	72	GLY	C-N-CA	5.41	128.07	120.28
1	C	62	MET	N-CA-C	-5.41	101.07	109.72
1	A	169	ASN	CA-C-N	5.39	131.98	121.41
1	A	169	ASN	C-N-CA	5.39	131.98	121.41
1	C	226	VAL	O-C-N	-5.39	117.44	123.26
1	C	340	ALA	N-CA-C	-5.36	105.52	111.36
1	C	216	GLY	O-C-N	5.35	127.94	123.29
1	D	155	GLY	CA-C-N	5.34	127.71	120.44
1	D	155	GLY	C-N-CA	5.34	127.71	120.44
1	B	132	ALA	N-CA-C	5.33	117.63	109.95
1	B	382	GLN	N-CA-C	-5.33	105.47	111.28
1	B	324	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	D	218	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	252	PHE	N-CA-C	5.30	117.14	111.36
1	B	373	GLN	N-CA-C	-5.29	107.38	113.88
1	B	218	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	375	TYR	N-CA-C	5.27	117.93	110.50
1	A	185	ASP	CA-C-N	5.25	125.06	119.28
1	A	185	ASP	C-N-CA	5.25	125.06	119.28
1	D	170	GLY	O-C-N	-5.23	116.78	122.54
1	A	218	ARG	NE-CZ-NH2	5.23	123.91	119.20
1	B	28	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	D	228	GLU	O-C-N	5.22	129.16	123.27
1	D	340	ALA	N-CA-C	-5.22	105.49	111.07
1	A	120	TYR	N-CA-C	5.20	118.09	111.69
1	A	194	PHE	N-CA-C	5.20	117.44	109.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	218	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	D	188	ALA	CA-C-N	5.16	125.16	119.89
1	D	188	ALA	C-N-CA	5.16	125.16	119.89
1	B	110	ILE	N-CA-C	5.14	116.61	111.00
1	A	210	ARG	NE-CZ-NH2	5.14	123.83	119.20
1	C	63	ASN	CB-CA-C	-5.13	102.87	111.23
1	A	234	LYS	N-CA-C	5.08	118.95	112.34
1	C	260	ALA	N-CA-C	-5.04	105.78	111.28
1	B	295	SER	N-CA-C	-5.04	105.78	111.28

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	ASN	Mainchain
1	A	229	ASP	Mainchain
1	A	230	VAL	Mainchain
1	B	285	GLY	Mainchain
1	B	29	LYS	Mainchain
1	C	217	GLN	Mainchain
1	C	218	ARG	Mainchain
1	C	269	ARG	Sidechain
1	D	181	ARG	Sidechain
1	D	217	GLN	Mainchain
1	D	218	ARG	Sidechain
1	D	223	ARG	Sidechain
1	D	229	ASP	Mainchain
1	D	309	ARG	Sidechain
1	D	367	ARG	Sidechain
1	D	55	ARG	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	2993	0	2982	132	0
1	B	2993	0	2981	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2993	0	2981	120	0
1	D	2993	0	2981	151	0
2	A	53	0	31	5	0
2	B	53	0	31	1	0
2	C	53	0	31	4	0
2	D	53	0	31	1	0
All	All	12184	0	12049	493	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (493) 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:137:GLU:HB2	1:D:138:PRO:CD	1.72	1.17
1:D:137:GLU:CB	1:D:138:PRO:HD2	1.90	1.01
1:A:197:PHE:HB3	1:A:237:VAL:HA	1.41	0.99
1:C:208:ILE:HG22	1:C:209:GLY:H	1.27	0.98
1:B:284:PHE:CZ	1:B:284:PHE:CD2	2.42	0.98
1:D:137:GLU:HB2	1:D:138:PRO:HD2	0.95	0.93
1:A:282:LYS:HG2	1:A:287:LEU:HD23	1.53	0.90
1:C:203:THR:HG23	1:C:204:PRO:HD2	1.56	0.88
1:C:62:MET:HG3	1:C:98:ILE:HG23	1.58	0.86
1:B:28:ARG:HG3	1:B:32:ARG:NH1	1.92	0.85
1:D:119:LYS:HA	1:D:123:ARG:NH2	1.92	0.83
1:A:304:LYS:HA	1:A:304:LYS:HZ2	1.43	0.83
1:A:304:LYS:HA	1:A:304:LYS:NZ	1.93	0.83
1:C:294:ILE:HD11	2:D:399:FAD:H1B	1.60	0.83
1:C:311:SER:OG	1:C:332:ALA:HA	1.79	0.81
1:A:281:ARG:HB3	1:A:288:LEU:HD12	1.63	0.81
1:B:49:PRO:HG3	1:B:94:VAL:HG12	1.63	0.81
1:C:101:ASN:HA	1:C:131:CYS:SG	2.24	0.77
1:A:36:ILE:HB	1:A:37:PRO:HD3	1.68	0.76
1:B:144:VAL:HG21	1:B:249:MET:HE1	1.66	0.75
1:A:143:ASP:OD1	1:A:143:ASP:O	2.05	0.75
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.68	0.75
1:A:112:GLY:O	1:A:117:LYS:HD2	1.86	0.74
1:C:374:ILE:HA	1:C:378:THR:HG22	1.69	0.74
1:C:269:ARG:HG2	1:C:269:ARG:HH11	1.51	0.74
1:C:387:ALA:O	1:C:391:ILE:HG12	1.88	0.73
1:D:309:ARG:O	1:D:313:GLN:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:PHE:HA	1:D:255:THR:OG1	1.89	0.72
1:C:234:LYS:O	1:C:237:VAL:HG22	1.89	0.72
1:D:381:ILE:HA	1:D:384:LEU:HD12	1.72	0.72
1:D:42:TYR:CE2	1:D:49:PRO:HA	2.25	0.71
1:B:28:ARG:CG	1:B:32:ARG:NH1	2.54	0.71
1:D:158:TYR:OH	1:D:241:ASP:HB2	1.91	0.70
1:B:132:ALA:HB3	1:B:176:TYR:HD1	1.55	0.70
1:D:113:ASN:O	1:D:117:LYS:HG3	1.91	0.70
1:A:156:ASP:HA	1:A:234:LYS:HG2	1.74	0.70
1:C:137:GLU:HG3	1:C:147:ILE:HG22	1.73	0.70
1:B:300:GLU:O	1:B:304:LYS:HG2	1.91	0.69
1:C:260:ALA:O	1:C:264:VAL:HG23	1.93	0.69
1:B:199:VAL:HG22	1:B:232:VAL:HG11	1.73	0.69
1:D:165:MET:HE3	1:D:166:TRP:H	1.57	0.69
1:A:289:VAL:HG21	1:D:391:ILE:HG12	1.75	0.69
1:B:233:PRO:HB2	1:B:235:GLU:HG2	1.74	0.69
1:A:62:MET:HG3	1:A:98:ILE:HG23	1.75	0.68
1:B:189:PRO:HB2	1:B:191:ASN:OD1	1.93	0.68
1:C:160:ILE:HG21	1:C:178:LEU:HD21	1.75	0.67
1:A:207:GLN:HB2	1:A:226:VAL:HG23	1.76	0.67
1:B:117:LYS:O	1:B:121:LEU:HB2	1.95	0.67
1:D:28:ARG:O	1:D:32:ARG:HG2	1.95	0.67
1:D:114:ASP:O	1:D:118:LYS:HG3	1.95	0.67
1:A:195:THR:HG23	1:A:195:THR:O	1.94	0.66
1:D:374:ILE:HA	1:D:378:THR:HG22	1.75	0.66
1:D:134:CYS:HA	1:D:167:ILE:HD12	1.78	0.66
1:D:263:ALA:HB2	1:D:372:TYR:CD2	2.31	0.66
1:A:209:GLY:O	1:A:223:ARG:HD3	1.96	0.66
1:A:264:VAL:HG11	1:A:309:ARG:HG3	1.78	0.66
1:B:27:ALA:HB1	1:B:86:GLU:HB2	1.78	0.66
1:D:137:GLU:CB	1:D:138:PRO:CD	2.52	0.66
1:B:171:GLY:HA2	1:B:208:ILE:HG21	1.78	0.65
1:C:111:ALA:HB1	1:C:239:ILE:HD11	1.77	0.65
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.78	0.65
1:C:215:MET:HB2	1:D:363:GLU:HG2	1.79	0.65
1:D:23:PHE:CZ	1:D:75:LEU:HD21	2.31	0.65
1:A:349:GLN:HE21	1:B:370:LYS:NZ	1.95	0.65
1:B:16:PHE:HE2	1:B:82:LEU:HD11	1.61	0.65
1:A:292:GLN:HB3	1:C:292:GLN:HB2	1.79	0.64
1:D:29:LYS:O	1:D:33:GLU:HB2	1.97	0.64
1:B:64:THR:HG22	1:B:75:LEU:HD22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:PHE:CD2	1:D:237:VAL:HG22	2.33	0.64
1:D:68:GLU:HA	1:D:72:GLY:O	1.98	0.64
1:B:108:ILE:HD12	1:B:198:ILE:HD11	1.80	0.63
1:D:152:GLU:HG3	1:D:159:ILE:HB	1.79	0.63
1:C:208:ILE:HG22	1:C:209:GLY:N	2.08	0.63
1:B:161:ASN:HD21	1:B:229:ASP:CG	2.07	0.63
1:A:50:VAL:HB	1:A:51:PRO:HD3	1.81	0.63
1:A:271:LEU:HD13	1:A:301:MET:HB3	1.80	0.63
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.64	0.63
1:A:362:VAL:HA	1:A:365:LEU:HD22	1.80	0.62
1:C:274:ALA:HB1	1:C:350:ILE:HD12	1.81	0.62
1:C:117:LYS:O	1:C:121:LEU:HB2	1.99	0.62
1:B:227:PHE:HD1	1:B:230:VAL:HG21	1.65	0.62
1:D:183:ASP:HB2	1:D:193:ALA:HA	1.80	0.62
1:A:218:ARG:HE	1:A:367:ARG:NH2	1.99	0.61
1:B:238:LEU:HD23	1:B:247:VAL:HG11	1.81	0.61
1:C:211:LYS:HA	1:C:223:ARG:HG2	1.81	0.61
1:D:217:GLN:NE2	1:D:371:ILE:HG21	2.15	0.61
1:B:150:LYS:O	1:B:160:ILE:HA	2.00	0.61
1:D:377:GLY:HA3	1:D:382:GLN:NE2	2.15	0.61
1:C:377:GLY:HA2	1:C:381:ILE:HD11	1.83	0.61
1:B:62:MET:HE3	1:B:101:ASN:ND2	2.15	0.61
1:C:105:GLN:O	1:C:108:ILE:HG12	2.00	0.60
1:A:197:PHE:HD2	1:A:237:VAL:HG22	1.66	0.60
1:B:106:MET:HE3	1:B:109:ILE:HB	1.84	0.60
1:A:374:ILE:HG12	1:B:349:GLN:HE22	1.65	0.60
1:D:34:GLU:OE1	1:D:34:GLU:HA	2.00	0.60
1:C:256:ARG:HH11	1:C:256:ARG:HG3	1.65	0.60
1:D:82:LEU:HD12	1:D:83:ILE:N	2.16	0.60
1:B:152:GLU:CG	1:B:154:LYS:HE2	2.32	0.60
1:A:298:LEU:HD23	1:D:391:ILE:HD11	1.83	0.59
1:C:134:CYS:HB3	1:C:164:LYS:HG3	1.84	0.59
1:D:137:GLU:OE2	1:D:147:ILE:HG23	2.02	0.59
1:B:101:ASN:O	1:B:105:GLN:HG3	2.02	0.59
1:D:62:MET:HE2	1:D:98:ILE:CG2	2.32	0.59
1:D:375:TYR:O	1:D:375:TYR:HD1	1.85	0.59
1:A:132:ALA:HB3	1:A:176:TYR:CD1	2.38	0.59
1:D:187:LYS:HD3	1:D:187:LYS:N	2.18	0.59
1:B:154:LYS:HG3	1:B:159:ILE:HD12	1.85	0.58
1:C:319:VAL:HB	1:C:325:ASN:ND2	2.19	0.58
1:B:173:ALA:HB3	1:B:176:TYR:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:HE2	1:B:339:ILE:HG22	1.86	0.58
1:C:305:VAL:HG23	1:C:343:LEU:HD21	1.86	0.58
1:D:324:ARG:NH2	1:D:326:THR:HG21	2.18	0.58
1:D:111:ALA:HB3	1:D:238:LEU:HD12	1.85	0.58
1:A:91:CYS:SG	1:A:94:VAL:HG23	2.44	0.57
1:A:147:ILE:HG13	1:A:147:ILE:O	2.02	0.57
1:B:249:MET:HA	1:B:252:PHE:CD2	2.39	0.57
1:B:27:ALA:HB3	1:B:86:GLU:HG3	1.85	0.57
1:D:268:GLN:HG2	1:D:305:VAL:HG21	1.86	0.57
1:A:139:GLY:HA2	1:B:281:ARG:HH12	1.67	0.57
1:D:279:LEU:O	1:D:287:LEU:HD22	2.04	0.57
1:A:195:THR:O	1:A:195:THR:CG2	2.52	0.57
1:C:138:PRO:HG3	1:C:165:MET:HE2	1.87	0.57
1:B:36:ILE:HD11	1:B:269:ARG:CZ	2.34	0.57
1:A:105:GLN:HG3	1:A:131:CYS:SG	2.44	0.57
1:B:277:TYR:CE2	1:B:351:LEU:HA	2.40	0.57
1:A:349:GLN:NE2	1:B:370:LYS:NZ	2.51	0.56
1:B:134:CYS:HA	1:B:167:ILE:HD12	1.86	0.56
1:A:147:ILE:HD11	1:A:179:LEU:HB3	1.88	0.56
1:A:168:THR:OG1	2:A:399:FAD:N5	2.37	0.56
1:A:212:GLU:HG2	1:A:223:ARG:HA	1.87	0.56
1:D:134:CYS:HA	1:D:167:ILE:CD1	2.35	0.56
1:A:181:ARG:HD2	1:A:183:ASP:O	2.06	0.56
1:C:38:VAL:CG2	1:C:52:LEU:HD11	2.36	0.56
1:C:55:ARG:O	1:C:59:LEU:HG	2.05	0.56
1:C:308:ALA:O	1:C:311:SER:HB3	2.05	0.56
1:C:227:PHE:CD1	1:C:227:PHE:N	2.74	0.56
1:B:152:GLU:HG3	1:B:154:LYS:HE2	1.87	0.56
1:D:40:ALA:O	1:D:44:LYS:HG2	2.06	0.56
1:B:297:MET:O	1:B:301:MET:HG3	2.06	0.56
2:A:399:FAD:H1B	1:B:294:ILE:HD11	1.88	0.55
1:B:151:ALA:HA	1:B:159:ILE:O	2.06	0.55
1:C:109:ILE:HD13	1:C:121:LEU:HD11	1.87	0.55
1:C:269:ARG:O	1:C:273:GLU:HG2	2.05	0.55
1:C:370:LYS:HD3	1:D:345:THR:HG23	1.87	0.55
1:B:144:VAL:O	1:B:147:ILE:HG23	2.06	0.55
1:A:246:LYS:NZ	1:A:246:LYS:HB3	2.22	0.55
1:C:376:GLU:HG3	1:C:376:GLU:O	2.06	0.55
1:A:147:ILE:CD1	1:A:179:LEU:HB3	2.37	0.55
1:D:117:LYS:O	1:D:121:LEU:HB2	2.06	0.55
1:A:171:GLY:HA2	1:A:208:ILE:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:PHE:CE2	1:B:82:LEU:HD11	2.42	0.54
1:C:208:ILE:CG2	1:C:209:GLY:H	2.05	0.54
1:B:238:LEU:CD2	1:B:247:VAL:HG11	2.38	0.54
1:D:82:LEU:HD12	1:D:83:ILE:HG13	1.90	0.54
1:B:282:LYS:HB3	1:B:287:LEU:HA	1.89	0.54
1:D:191:ASN:ND2	1:D:192:LYS:HG3	2.22	0.54
1:A:279:LEU:HD23	1:A:289:VAL:HG11	1.88	0.54
1:B:325:ASN:ND2	1:B:329:ALA:HB2	2.23	0.54
1:C:34:GLU:O	1:C:38:VAL:HG22	2.08	0.54
1:A:289:VAL:CG2	1:D:391:ILE:HG12	2.37	0.54
1:D:108:ILE:HA	1:D:238:LEU:HD11	1.88	0.54
1:D:311:SER:O	1:D:332:ALA:HB2	2.08	0.53
1:D:319:VAL:HB	1:D:325:ASN:ND2	2.22	0.53
1:C:203:THR:HG21	1:C:230:VAL:HG13	1.91	0.53
1:B:106:MET:HE2	1:B:110:ILE:HG23	1.91	0.53
1:D:49:PRO:HG2	1:D:53:ILE:HD11	1.91	0.53
1:D:264:VAL:HG11	1:D:312:TYR:HE2	1.72	0.53
1:B:26:THR:HG22	1:B:61:LEU:HD21	1.89	0.53
2:C:399:FAD:H1B	1:D:294:ILE:HD11	1.90	0.53
1:D:362:VAL:HA	1:D:365:LEU:HG	1.89	0.53
1:C:164:LYS:HB3	1:C:167:ILE:HD11	1.90	0.53
1:B:309:ARG:HA	1:B:312:TYR:CE2	2.42	0.53
1:A:191:ASN:HB3	1:A:192:LYS:HG3	1.91	0.53
1:A:374:ILE:HG12	1:B:349:GLN:NE2	2.24	0.53
1:B:36:ILE:HG22	1:B:37:PRO:HD3	1.91	0.53
1:B:292:GLN:HE21	1:C:384:LEU:HD21	1.74	0.53
1:A:77:THR:HG23	1:A:254:LYS:HE2	1.90	0.53
1:B:32:ARG:HG3	1:B:32:ARG:HH11	1.74	0.53
1:C:62:MET:HE3	1:C:101:ASN:ND2	2.24	0.53
1:C:166:TRP:CZ3	1:C:212:GLU:HG2	2.44	0.53
1:C:349:GLN:HE21	1:D:370:LYS:NZ	2.07	0.52
1:C:50:VAL:HB	1:C:51:PRO:HD3	1.91	0.52
1:A:32:ARG:HA	1:A:36:ILE:HD12	1.91	0.52
1:D:119:LYS:HA	1:D:123:ARG:HH21	1.69	0.52
1:D:181:ARG:HH22	1:D:186:PRO:HA	1.74	0.52
1:B:292:GLN:HB3	1:D:292:GLN:HB3	1.92	0.52
1:C:28:ARG:HG3	1:C:32:ARG:NE	2.24	0.52
1:C:112:GLY:O	1:C:117:LYS:HE3	2.09	0.52
1:D:283:THR:HG21	1:D:288:LEU:HD21	1.92	0.52
1:B:28:ARG:HG3	1:B:32:ARG:HH12	1.71	0.52
1:A:390:HIS:HA	1:A:393:LYS:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:THR:CG2	1:B:75:LEU:HD22	2.39	0.52
1:B:299:ALA:O	1:B:303:MET:HG3	2.10	0.52
1:D:198:ILE:HG22	1:D:236:ASN:O	2.10	0.52
1:A:113:ASN:OD1	1:A:115:GLN:HB2	2.10	0.52
1:B:19:GLN:O	1:B:22:GLU:HG2	2.10	0.52
1:D:150:LYS:HE2	1:D:184:PRO:HB3	1.92	0.52
1:D:311:SER:OG	1:D:332:ALA:HA	2.10	0.52
1:A:136:THR:HG23	1:A:141:GLY:HA2	1.92	0.51
1:D:32:ARG:HA	1:D:36:ILE:HD12	1.92	0.51
1:D:181:ARG:HH12	1:D:186:PRO:HA	1.75	0.51
1:D:300:GLU:HA	1:D:303:MET:HG2	1.93	0.51
1:B:24:GLN:O	1:B:27:ALA:HB3	2.11	0.51
1:C:207:GLN:HB2	1:C:226:VAL:CG2	2.40	0.51
1:A:141:GLY:HA3	2:A:399:FAD:O2P	2.11	0.51
1:B:27:ALA:HB1	1:B:86:GLU:CB	2.41	0.51
1:B:325:ASN:HD21	1:B:329:ALA:HB2	1.75	0.51
1:A:249:MET:HA	1:A:249:MET:HE3	1.92	0.51
1:C:85:GLU:HG3	1:C:265:GLY:HA2	1.93	0.51
1:B:49:PRO:HD3	1:B:219:CYS:HB2	1.93	0.51
1:C:207:GLN:HB2	1:C:226:VAL:HG22	1.93	0.51
1:D:187:LYS:HD3	1:D:187:LYS:H	1.76	0.51
1:D:215:MET:HG2	1:D:215:MET:O	2.11	0.51
1:D:390:HIS:HD2	1:D:391:ILE:HD12	1.74	0.51
1:B:36:ILE:HD12	1:B:90:GLY:HA2	1.92	0.51
1:D:197:PHE:HB3	1:D:232:VAL:HG11	1.92	0.51
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.93	0.51
1:B:141:GLY:HA3	2:B:399:FAD:O2P	2.11	0.51
1:C:266:LEU:HD11	1:C:365:LEU:HB3	1.92	0.51
1:A:178:LEU:O	1:A:196:GLY:HA2	2.11	0.50
1:A:281:ARG:HB3	1:A:288:LEU:CD1	2.38	0.50
1:B:27:ALA:CB	1:B:86:GLU:HG3	2.40	0.50
1:B:304:LYS:O	1:B:339:ILE:HD13	2.10	0.50
1:C:38:VAL:HG21	1:C:52:LEU:HD11	1.93	0.50
1:C:252:PHE:O	1:C:256:ARG:HG2	2.11	0.50
1:C:379:SER:HB3	1:C:383:ARG:NH1	2.26	0.50
1:D:333:LYS:HG2	1:D:382:GLN:NE2	2.26	0.50
1:D:73:LEU:HG	1:D:75:LEU:HD13	1.94	0.50
1:A:387:ALA:HB2	1:D:299:ALA:HB2	1.93	0.50
1:B:161:ASN:ND2	1:B:229:ASP:H	2.10	0.50
1:D:215:MET:O	1:D:215:MET:CG	2.60	0.49
1:A:207:GLN:HB2	1:A:226:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:ALA:HB1	1:C:366:MET:HA	1.94	0.49
1:B:210:ARG:HG2	1:B:211:LYS:N	2.27	0.49
1:D:42:TYR:HB3	1:D:219:CYS:HB3	1.94	0.49
1:A:362:VAL:HA	1:A:365:LEU:CD2	2.43	0.49
1:C:342:GLN:O	1:C:345:THR:HG22	2.13	0.49
1:A:53:ILE:HG22	1:A:62:MET:SD	2.52	0.49
1:C:395:LYS:O	1:C:396:ASN:HB2	2.12	0.49
1:A:137:GLU:HG2	1:A:164:LYS:HD3	1.94	0.49
1:A:279:LEU:HD21	1:D:391:ILE:HG23	1.95	0.49
1:B:306:GLU:O	1:B:310:MET:HE3	2.13	0.49
1:C:91:CYS:SG	1:C:94:VAL:HG23	2.53	0.49
1:A:370:LYS:HB3	1:B:356:PHE:HE1	1.78	0.49
1:A:105:GLN:O	1:A:109:ILE:HG13	2.12	0.49
1:B:136:THR:HG23	1:B:140:ALA:O	2.13	0.49
1:C:377:GLY:CA	1:C:381:ILE:HD11	2.42	0.49
1:D:41:GLU:O	1:D:45:THR:HG23	2.13	0.49
1:B:292:GLN:HB3	1:D:292:GLN:CB	2.43	0.48
1:C:266:LEU:HD21	1:C:369:ALA:HB2	1.93	0.48
1:D:36:ILE:HB	1:D:37:PRO:HD3	1.95	0.48
1:D:168:THR:HG22	1:D:169:ASN:HD22	1.78	0.48
1:D:210:ARG:NH2	1:D:213:LEU:HD23	2.28	0.48
1:D:197:PHE:CE2	1:D:237:VAL:HG22	2.48	0.48
1:A:130:MET:HG3	1:A:169:ASN:OD1	2.13	0.48
1:C:153:LYS:HG2	1:C:158:TYR:CE2	2.48	0.48
1:C:164:LYS:HE3	1:C:178:LEU:CD1	2.43	0.48
1:A:159:ILE:CD1	1:A:231:LYS:HG2	2.43	0.48
1:A:177:PHE:CZ	1:A:248:ALA:HB2	2.49	0.48
1:C:216:GLY:O	1:C:217:GLN:C	2.56	0.48
1:A:101:ASN:OD1	1:A:130:MET:HA	2.13	0.48
1:A:210:ARG:O	1:A:223:ARG:HB2	2.14	0.48
1:C:388:ARG:HD2	1:C:388:ARG:C	2.37	0.48
1:A:99:GLU:OE2	1:A:258:VAL:HG11	2.13	0.48
1:C:191:ASN:HA	1:C:245:PHE:HB3	1.96	0.48
1:C:297:MET:O	1:C:301:MET:HG3	2.13	0.48
1:A:243:ALA:O	1:A:247:VAL:HG23	2.14	0.48
1:D:264:VAL:HG11	1:D:312:TYR:CE2	2.47	0.48
1:A:349:GLN:NE2	1:B:370:LYS:HZ3	2.12	0.48
1:C:176:TYR:HE1	1:C:201:ALA:HA	1.79	0.48
1:D:210:ARG:HH21	1:D:213:LEU:HD23	1.78	0.48
1:C:18:GLU:OE1	1:C:21:LYS:HD2	2.14	0.47
1:C:277:TYR:O	1:C:280:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:ASP:OD1	1:D:187:LYS:HE3	2.14	0.47
1:D:134:CYS:SG	1:D:225:ILE:HD12	2.54	0.47
1:C:101:ASN:O	1:C:131:CYS:SG	2.73	0.47
1:A:89:TYR:O	1:A:269:ARG:HD3	2.14	0.47
1:D:65:HIS:O	1:D:66:ILE:C	2.56	0.47
1:A:245:PHE:O	1:A:249:MET:HB2	2.15	0.47
1:B:28:ARG:O	1:B:29:LYS:C	2.58	0.47
1:B:123:ARG:HH11	1:B:174:ASN:ND2	2.13	0.47
1:B:333:LYS:HD2	1:B:333:LYS:O	2.15	0.47
1:C:256:ARG:HB2	1:C:257:PRO:HD3	1.97	0.47
1:B:32:ARG:NH1	1:B:32:ARG:HG3	2.30	0.47
1:A:303:MET:O	1:A:307:LEU:HD22	2.15	0.47
1:D:150:LYS:HG3	1:D:181:ARG:O	2.15	0.47
1:A:342:GLN:O	1:A:345:THR:HG22	2.14	0.47
1:D:252:PHE:HA	1:D:255:THR:CB	2.44	0.47
1:A:335:PHE:O	1:A:339:ILE:HG23	2.15	0.46
1:A:267:ALA:HB1	1:A:343:LEU:HD22	1.97	0.46
1:C:282:LYS:HA	1:C:287:LEU:HA	1.97	0.46
1:D:101:ASN:HA	1:D:131:CYS:SG	2.55	0.46
1:D:208:ILE:HG22	1:D:225:ILE:HG23	1.96	0.46
1:A:370:LYS:HB3	1:B:356:PHE:CE1	2.51	0.46
1:D:35:ILE:HG12	1:D:52:LEU:HD13	1.97	0.46
1:D:157:GLU:HA	1:D:234:LYS:HB2	1.97	0.46
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.50	0.46
1:A:167:ILE:HG22	1:A:170:GLY:H	1.81	0.46
1:C:66:ILE:HG12	1:C:121:LEU:HD22	1.98	0.46
1:C:388:ARG:HD2	1:C:388:ARG:O	2.16	0.46
1:A:357:ASN:HB2	1:B:166:TRP:CH2	2.51	0.46
1:B:317:TRP:CZ3	1:C:14:PHE:HB2	2.51	0.46
1:B:358:THR:C	1:B:360:TYR:H	2.23	0.46
1:D:303:MET:O	1:D:307:LEU:HD13	2.16	0.46
1:B:161:ASN:HA	1:B:227:PHE:O	2.16	0.46
1:C:256:ARG:O	1:C:259:VAL:HG12	2.16	0.46
1:D:266:LEU:CD1	1:D:369:ALA:HB2	2.46	0.46
1:D:318:GLU:OE1	1:D:323:ARG:HD2	2.15	0.46
1:D:327:TYR:HD1	1:D:389:GLU:HB3	1.80	0.46
1:B:190:ALA:HA	1:B:193:ALA:HB3	1.98	0.46
1:C:380:GLN:HB2	2:C:399:FAD:O2B	2.16	0.46
1:D:57:TRP:CZ2	1:D:128:PRO:HD3	2.51	0.46
1:B:132:ALA:HB3	1:B:176:TYR:CD1	2.43	0.45
1:B:394:TYR:HB2	1:C:279:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:PHE:CE1	1:C:237:VAL:HG12	2.51	0.45
1:D:105:GLN:HG3	1:D:131:CYS:SG	2.55	0.45
1:D:132:ALA:HB3	1:D:176:TYR:HD1	1.80	0.45
1:B:62:MET:HG3	1:B:98:ILE:HG23	1.97	0.45
1:C:203:THR:CG2	1:C:230:VAL:HG13	2.47	0.45
1:B:231:LYS:O	1:B:231:LYS:HG2	2.16	0.45
1:A:49:PRO:HD3	1:A:219:CYS:HB2	1.98	0.45
1:A:92:THR:HA	1:A:95:GLN:HB3	1.98	0.45
1:D:159:ILE:CD1	1:D:231:LYS:HG3	2.47	0.45
1:D:301:MET:HE1	1:D:350:ILE:HD12	1.99	0.45
1:D:351:LEU:HD22	1:D:362:VAL:HG22	1.98	0.45
1:A:106:MET:HB3	1:A:107:PRO:HD3	1.99	0.45
1:B:165:MET:HE3	1:B:166:TRP:CD2	2.52	0.45
1:B:299:ALA:HB2	1:C:387:ALA:HB2	1.98	0.45
1:C:42:TYR:CE1	1:C:49:PRO:HA	2.52	0.45
1:D:53:ILE:HG23	1:D:62:MET:HE1	1.98	0.45
1:D:344:ALA:O	1:D:348:VAL:HG23	2.17	0.45
1:D:344:ALA:HB1	1:D:366:MET:HA	1.97	0.45
1:C:358:THR:HB	1:D:213:LEU:O	2.17	0.45
1:D:228:GLU:O	1:D:228:GLU:HG3	2.17	0.45
1:A:381:ILE:HG23	1:A:384:LEU:HD12	1.98	0.45
1:C:197:PHE:CD1	1:C:237:VAL:HG12	2.52	0.45
1:C:327:TYR:O	1:C:331:ILE:HG23	2.16	0.45
1:D:142:SER:HB2	1:D:381:ILE:HG21	1.99	0.45
1:D:206:ILE:HG12	1:D:227:PHE:CD1	2.52	0.45
1:C:10:LEU:HD12	1:C:11:GLY:H	1.81	0.45
1:C:164:LYS:HE3	1:C:178:LEU:HD11	1.98	0.45
1:C:286:LYS:HB2	1:C:290:GLU:OE2	2.16	0.45
1:D:115:GLN:HA	1:D:118:LYS:NZ	2.31	0.45
1:B:279:LEU:HD23	1:B:289:VAL:HG11	1.98	0.44
1:D:109:ILE:HG12	1:D:121:LEU:HD21	1.98	0.44
1:A:304:LYS:HB3	1:A:339:ILE:HD12	1.98	0.44
1:B:325:ASN:ND2	1:B:329:ALA:CB	2.80	0.44
1:B:294:ILE:HA	1:B:297:MET:HG3	1.99	0.44
1:B:181:ARG:HA	1:B:194:PHE:HD1	1.82	0.44
1:D:111:ALA:HB1	1:D:239:ILE:HG13	1.98	0.44
1:D:351:LEU:HD22	1:D:362:VAL:CG2	2.48	0.44
1:A:339:ILE:HG13	1:A:340:ALA:N	2.31	0.44
1:C:168:THR:O	1:C:169:ASN:HB2	2.18	0.44
1:A:85:GLU:HB2	1:A:261:ALA:HB1	1.99	0.44
1:D:326:THR:HG23	1:D:327:TYR:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:ALA:O	1:A:351:LEU:HD13	2.17	0.44
1:A:356:PHE:CE1	1:B:215:MET:HE2	2.53	0.44
1:B:174:ASN:HD22	1:B:175:TRP:HD1	1.66	0.44
1:D:149:THR:HG23	1:D:162:GLY:HA3	2.00	0.44
1:A:314:ARG:HD2	1:D:14:PHE:CD2	2.53	0.44
1:B:122:GLY:O	1:B:125:THR:HB	2.18	0.44
1:D:157:GLU:HB2	1:D:232:VAL:O	2.18	0.44
1:A:124:MET:HE3	1:A:175:TRP:HE1	1.83	0.43
1:A:356:PHE:CD2	1:B:214:ASN:HB3	2.53	0.43
1:A:190:ALA:HB1	1:A:245:PHE:CE1	2.53	0.43
1:A:287:LEU:O	1:A:290:GLU:HB2	2.19	0.43
1:B:62:MET:HE3	1:B:101:ASN:HD22	1.83	0.43
1:A:282:LYS:HB2	1:A:282:LYS:NZ	2.33	0.43
1:C:239:ILE:HB	1:C:243:ALA:CB	2.48	0.43
1:A:109:ILE:HG12	1:A:121:LEU:HD11	2.00	0.43
1:A:189:PRO:O	1:A:190:ALA:C	2.61	0.43
1:B:110:ILE:HG13	1:B:111:ALA:N	2.33	0.43
1:A:354:ASN:HB3	1:A:360:TYR:CE2	2.52	0.43
1:C:42:TYR:HD1	1:C:47:GLU:HG3	1.83	0.43
1:D:173:ALA:HB3	1:D:176:TYR:CE1	2.53	0.43
1:A:113:ASN:OD1	1:A:113:ASN:C	2.61	0.43
1:A:133:TYR:CE2	1:A:135:VAL:HG21	2.54	0.43
1:B:325:ASN:HD21	1:B:329:ALA:CB	2.32	0.43
2:C:399:FAD:H2B	2:C:399:FAD:H52A	1.78	0.43
1:D:382:GLN:OE1	1:D:382:GLN:HA	2.19	0.43
1:A:211:LYS:HA	1:A:223:ARG:HB3	2.01	0.43
1:A:385:ILE:O	1:A:388:ARG:HB3	2.19	0.43
1:B:131:CYS:HA	1:B:173:ALA:HB1	2.01	0.43
1:D:30:PHE:CE1	1:D:34:GLU:HB2	2.53	0.43
1:B:126:GLU:H	1:B:126:GLU:HG2	1.70	0.43
1:D:108:ILE:HD11	1:D:198:ILE:HD13	2.00	0.43
1:D:183:ASP:HA	1:D:184:PRO:HD2	1.90	0.43
1:A:88:ALA:HB2	1:A:95:GLN:HG3	2.01	0.43
1:A:157:GLU:C	1:A:158:TYR:HD1	2.27	0.43
1:C:143:ASP:HA	1:D:284:PHE:CZ	2.54	0.43
1:A:142:SER:H	2:A:399:FAD:H5'2	1.84	0.42
1:A:159:ILE:C	1:A:160:ILE:HD12	2.43	0.42
1:C:364:LYS:O	1:C:364:LYS:HD3	2.19	0.42
1:C:267:ALA:HB1	1:C:343:LEU:HD22	2.01	0.42
1:C:339:ILE:HD12	1:C:339:ILE:C	2.44	0.42
1:D:78:PHE:HA	1:D:316:ALA:HB1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:375:TYR:CD1	1:D:375:TYR:C	2.97	0.42
1:A:144:VAL:C	1:A:146:GLY:H	2.28	0.42
1:A:218:ARG:NE	1:A:367:ARG:NH2	2.65	0.42
1:A:234:LYS:O	1:A:237:VAL:HG23	2.20	0.42
1:B:36:ILE:HD11	1:B:269:ARG:NH1	2.35	0.42
1:B:238:LEU:HD12	1:B:238:LEU:HA	1.50	0.42
1:C:42:TYR:CD1	1:C:47:GLU:HG3	2.54	0.42
1:A:177:PHE:HZ	1:A:248:ALA:HB2	1.84	0.42
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.54	0.42
1:B:256:ARG:NE	1:B:382:GLN:HE22	2.18	0.42
1:C:180:ALA:O	1:C:194:PHE:HA	2.19	0.42
1:D:106:MET:HE2	1:D:254:LYS:HG3	2.01	0.42
1:A:185:ASP:HA	1:A:186:PRO:HD2	1.87	0.42
1:A:303:MET:HE3	1:A:303:MET:HB2	1.90	0.42
1:C:156:ASP:HA	1:C:234:LYS:HE2	2.01	0.42
2:C:399:FAD:N6A	1:D:291:HIS:CE1	2.87	0.42
1:D:145:ALA:HA	1:D:194:PHE:CZ	2.54	0.42
1:A:314:ARG:HD3	1:D:310:MET:SD	2.60	0.42
1:B:123:ARG:HH11	1:B:174:ASN:HD21	1.67	0.42
1:C:31:ALA:O	1:C:35:ILE:HB	2.19	0.42
1:C:203:THR:CG2	1:C:204:PRO:HD2	2.40	0.42
1:C:89:TYR:CE1	1:C:269:ARG:HA	2.55	0.42
1:C:267:ALA:HB1	1:C:343:LEU:CD2	2.49	0.42
1:D:54:ARG:O	1:D:57:TRP:HB3	2.20	0.42
1:D:137:GLU:HB3	1:D:164:LYS:HA	2.01	0.42
1:B:28:ARG:HG2	1:B:32:ARG:NH1	2.32	0.42
1:A:273:GLU:OE1	1:A:273:GLU:HA	2.20	0.42
1:C:122:GLY:O	1:C:125:THR:HB	2.20	0.42
1:C:382:GLN:HE21	1:C:382:GLN:HA	1.84	0.42
1:A:17:THR:HG22	1:A:20:GLN:HG3	2.02	0.41
1:A:208:ILE:O	1:A:208:ILE:HG22	2.20	0.41
1:C:103:LEU:O	1:C:107:PRO:HD2	2.20	0.41
1:C:266:LEU:O	1:C:266:LEU:HD12	2.20	0.41
1:C:319:VAL:HB	1:C:325:ASN:CG	2.44	0.41
1:D:119:LYS:HG2	1:D:119:LYS:O	2.19	0.41
1:D:161:ASN:HA	1:D:227:PHE:O	2.20	0.41
1:B:171:GLY:CA	1:B:208:ILE:HG21	2.50	0.41
1:B:194:PHE:O	1:B:242:GLY:C	2.63	0.41
1:B:281:ARG:HG3	1:B:288:LEU:HD13	2.02	0.41
1:C:375:TYR:CD1	1:C:375:TYR:C	2.96	0.41
1:D:55:ARG:HG3	1:D:55:ARG:HH11	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ASN:ND2	1:A:101:ASN:HB3	2.35	0.41
1:A:168:THR:O	1:A:169:ASN:HB2	2.20	0.41
1:C:382:GLN:O	1:C:386:VAL:HG23	2.19	0.41
1:D:66:ILE:HG22	1:D:72:GLY:HA3	2.00	0.41
1:A:373:GLN:HB3	1:B:349:GLN:OE1	2.21	0.41
1:C:239:ILE:HB	1:C:243:ALA:HB3	2.03	0.41
1:D:122:GLY:HA2	1:D:125:THR:OG1	2.19	0.41
1:A:69:ASN:C	1:A:71:GLY:H	2.29	0.41
1:B:282:LYS:HB3	1:B:287:LEU:HD23	2.01	0.41
1:C:181:ARG:NH2	1:C:188:ALA:HB3	2.36	0.41
1:D:319:VAL:HA	1:D:323:ARG:O	2.19	0.41
1:A:12:PHE:CE2	1:D:14:PHE:HA	2.55	0.41
1:A:189:PRO:HB2	1:A:191:ASN:HB2	2.03	0.41
1:B:249:MET:HA	1:B:252:PHE:HD2	1.86	0.41
1:D:17:THR:O	1:D:21:LYS:HG3	2.19	0.41
1:A:120:TYR:O	1:A:124:MET:HG2	2.20	0.41
1:D:87:LEU:HD13	1:D:98:ILE:HD11	2.01	0.41
1:A:134:CYS:HB2	1:A:178:LEU:HD12	2.03	0.41
1:A:355:GLY:O	1:A:363:GLU:HB2	2.21	0.41
1:C:371:ILE:HB	1:D:356:PHE:CZ	2.55	0.41
1:D:17:THR:OG1	1:D:20:GLN:HG3	2.21	0.41
1:D:160:ILE:HB	1:D:230:VAL:HB	2.03	0.41
1:A:18:GLU:H	1:D:10:LEU:HD12	1.85	0.41
1:A:190:ALA:HB1	1:A:245:PHE:CD1	2.56	0.41
2:A:399:FAD:H2B	2:A:399:FAD:H52A	1.78	0.41
1:B:36:ILE:HG22	1:B:37:PRO:CD	2.50	0.41
1:B:288:LEU:HA	1:B:291:HIS:ND1	2.35	0.41
1:C:40:ALA:O	1:C:44:LYS:HG3	2.21	0.41
1:C:185:ASP:HA	1:C:186:PRO:HD3	1.91	0.41
1:D:249:MET:HA	1:D:252:PHE:CZ	2.56	0.41
1:D:282:LYS:HD3	1:D:287:LEU:HD23	2.03	0.41
1:B:134:CYS:HB3	1:B:164:LYS:HG3	2.03	0.41
1:B:377:GLY:HA3	1:B:382:GLN:HE21	1.86	0.41
1:D:55:ARG:HH11	1:D:55:ARG:CG	2.34	0.41
1:A:154:LYS:HG2	1:A:154:LYS:O	2.22	0.40
1:A:235:GLU:CD	1:A:235:GLU:H	2.28	0.40
1:B:152:GLU:HG2	1:B:154:LYS:HE2	2.02	0.40
1:C:55:ARG:CZ	1:C:59:LEU:HD21	2.51	0.40
1:C:85:GLU:OE1	1:C:309:ARG:HD2	2.21	0.40
1:D:266:LEU:HD12	1:D:369:ALA:HB2	2.02	0.40
1:A:183:ASP:OD1	1:A:185:ASP:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:ALA:O	1:B:348:VAL:HG23	2.21	0.40
1:C:17:THR:HB	1:C:20:GLN:HG3	2.03	0.40
1:A:30:PHE:HD2	1:A:87:LEU:HD21	1.87	0.40
1:D:370:LYS:NZ	1:D:373:GLN:NE2	2.69	0.40
1:A:150:LYS:HD2	1:A:150:LYS:HA	1.87	0.40
1:A:166:TRP:CH2	1:B:357:ASN:HB2	2.57	0.40
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.87	0.40
1:C:328:TYR:O	1:C:331:ILE:HG12	2.21	0.40
1:C:334:ALA:HB2	1:C:382:GLN:HB3	2.03	0.40
1:D:50:VAL:HB	1:D:51:PRO:CD	2.51	0.40
1:D:186:PRO:HB2	1:D:187:LYS:HD3	2.03	0.40
1:D:256:ARG:HB2	1:D:257:PRO:HD3	2.03	0.40
1:D:389:GLU:O	1:D:393:LYS:HG3	2.20	0.40
1:A:59:LEU:HB3	1:A:61:LEU:HD23	2.03	0.40
1:C:373:GLN:O	1:C:374:ILE:HD13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/396 (97%)	343 (89%)	38 (10%)	4 (1%)	12	24
1	B	385/396 (97%)	349 (91%)	34 (9%)	2 (0%)	24	43
1	C	385/396 (97%)	355 (92%)	29 (8%)	1 (0%)	36	56
1	D	385/396 (97%)	347 (90%)	33 (9%)	5 (1%)	9	18
All	All	1540/1584 (97%)	1394 (90%)	134 (9%)	12 (1%)	16	30

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	141	GLY
1	B	326	THR
1	D	16	PHE
1	A	145	ALA
1	C	208	ILE
1	D	326	THR
1	A	114	ASP
1	A	16	PHE
1	D	145	ALA
1	D	238	LEU
1	A	142	SER
1	D	135	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/311 (98%)	267 (88%)	37 (12%)	5	8
1	B	304/311 (98%)	280 (92%)	24 (8%)	11	21
1	C	304/311 (98%)	275 (90%)	29 (10%)	8	16
1	D	304/311 (98%)	274 (90%)	30 (10%)	7	15
All	All	1216/1244 (98%)	1096 (90%)	120 (10%)	7	15

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	17	THR
1	A	41	GLU
1	A	77	THR
1	A	85	GLU
1	A	102	SER
1	A	127	GLU
1	A	142	SER
1	A	143	ASP
1	A	149	THR

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Mol	Chain	Res	Type
1	A	152	GLU
1	A	158	TYR
1	A	161	ASN
1	A	179	LEU
1	A	191	ASN
1	A	197	PHE
1	A	208	ILE
1	A	218	ARG
1	A	234	LYS
1	A	235	GLU
1	A	238	LEU
1	A	246	LYS
1	A	249	MET
1	A	253	ASP
1	A	258	VAL
1	A	282	LYS
1	A	283	THR
1	A	295	SER
1	A	296	PHE
1	A	304	LYS
1	A	307	LEU
1	A	333	LYS
1	A	365	LEU
1	A	366	MET
1	A	375	TYR
1	A	376	GLU
1	A	379	SER
1	B	28	ARG
1	B	36	ILE
1	B	55	ARG
1	B	64	THR
1	B	95	GLN
1	B	137	GLU
1	B	142	SER
1	B	160	ILE
1	B	185	ASP
1	B	197	PHE
1	B	207	GLN
1	B	210	ARG
1	B	211	LYS
1	B	218	ARG
1	B	231	LYS

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Mol	Chain	Res	Type
1	B	232	VAL
1	B	238	LEU
1	B	255	THR
1	B	297	MET
1	B	300	GLU
1	B	324	ARG
1	B	359	GLU
1	B	371	ILE
1	B	375	TYR
1	C	41	GLU
1	C	61	LEU
1	C	75	LEU
1	C	103	LEU
1	C	118	LYS
1	C	126	GLU
1	C	129	LEU
1	C	137	GLU
1	C	152	GLU
1	C	176	TYR
1	C	179	LEU
1	C	185	ASP
1	C	203	THR
1	C	207	GLN
1	C	212	GLU
1	C	221	ASP
1	C	222	THR
1	C	225	ILE
1	C	227	PHE
1	C	249	MET
1	C	266	LEU
1	C	282	LYS
1	C	298	LEU
1	C	305	VAL
1	C	309	ARG
1	C	358	THR
1	C	365	LEU
1	C	368	ASP
1	C	375	TYR
1	D	24	GLN
1	D	47	GLU
1	D	54	ARG
1	D	55	ARG

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Mol	Chain	Res	Type
1	D	75	LEU
1	D	94	VAL
1	D	96	THR
1	D	102	SER
1	D	117	LYS
1	D	137	GLU
1	D	154	LYS
1	D	157	GLU
1	D	178	LEU
1	D	179	LEU
1	D	187	LYS
1	D	198	ILE
1	D	210	ARG
1	D	218	ARG
1	D	223	ARG
1	D	234	LYS
1	D	254	LYS
1	D	269	ARG
1	D	282	LYS
1	D	295	SER
1	D	333	LYS
1	D	343	LEU
1	D	365	LEU
1	D	375	TYR
1	D	381	ILE
1	D	389	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	105	GLN
1	A	116	GLN
1	A	161	ASN
1	A	191	ASN
1	A	207	GLN
1	A	217	GLN
1	A	341	ASN
1	A	342	GLN
1	A	349	GLN
1	A	354	ASN
1	A	373	GLN

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Mol	Chain	Res	Type
1	A	396	ASN
1	B	65	HIS
1	B	95	GLN
1	B	161	ASN
1	B	169	ASN
1	B	174	ASN
1	B	268	GLN
1	B	325	ASN
1	B	354	ASN
1	B	396	ASN
1	C	69	ASN
1	C	115	GLN
1	C	161	ASN
1	C	292	GLN
1	C	313	GLN
1	C	349	GLN
1	C	382	GLN
1	C	396	ASN
1	D	20	GLN
1	D	95	GLN
1	D	207	GLN
1	D	217	GLN
1	D	357	ASN
1	D	373	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	A	399	-	58,58,58	1.34	7 (12%)	85,89,89	1.50	12 (14%)
2	FAD	B	399	-	58,58,58	1.61	6 (10%)	85,89,89	1.61	11 (12%)
2	FAD	C	399	-	58,58,58	1.27	4 (6%)	85,89,89	1.45	11 (12%)
2	FAD	D	399	-	58,58,58	1.69	8 (13%)	85,89,89	1.81	16 (18%)

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	A	399	-	-	5/34/50/50	0/6/6/6
2	FAD	B	399	-	-	9/34/50/50	0/6/6/6
2	FAD	C	399	-	-	8/34/50/50	0/6/6/6
2	FAD	D	399	-	-	9/34/50/50	0/6/6/6

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	FAD	PA-O3P	-7.58	1.51	1.59
2	D	399	FAD	PA-O3P	-6.78	1.52	1.59
2	C	399	FAD	C9-C8	-4.29	1.33	1.39
2	D	399	FAD	C6-C7	-4.15	1.34	1.39
2	B	399	FAD	P-O3P	-3.95	1.55	1.59
2	C	399	FAD	P-O3P	3.66	1.63	1.59
2	D	399	FAD	C5X-N5	-3.45	1.33	1.39
2	B	399	FAD	C4X-N5	3.41	1.38	1.30
2	D	399	FAD	C1B-N9A	3.37	1.55	1.46
2	A	399	FAD	C4X-N5	3.26	1.37	1.30
2	D	399	FAD	C9-C8	-3.21	1.35	1.39
2	C	399	FAD	C4X-N5	3.16	1.37	1.30
2	A	399	FAD	C6-C7	-3.13	1.35	1.39
2	A	399	FAD	C9-C8	-3.11	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	399	FAD	C10-N10	3.03	1.43	1.37
2	D	399	FAD	C10-N10	2.95	1.43	1.37
2	A	399	FAD	C10-N10	2.88	1.43	1.37
2	B	399	FAD	C6-C7	-2.79	1.35	1.39
2	B	399	FAD	C9-C8	-2.74	1.35	1.39
2	D	399	FAD	C4X-N5	2.55	1.36	1.30
2	A	399	FAD	C1'-N10	-2.46	1.41	1.47
2	B	399	FAD	C10-N10	2.44	1.42	1.37
2	A	399	FAD	C2-N3	-2.41	1.33	1.39
2	A	399	FAD	C10-N1	2.08	1.37	1.33
2	D	399	FAD	O4B-C1B	2.06	1.46	1.42

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	399	FAD	O3'-C3'-C2'	-5.90	95.52	108.93
2	B	399	FAD	C9A-C5X-N5	5.39	128.17	122.45
2	C	399	FAD	C2B-C3B-C4B	-5.07	92.82	102.61
2	D	399	FAD	C9A-C5X-N5	4.86	127.61	122.45
2	D	399	FAD	O3'-C3'-C2'	4.42	118.98	108.93
2	D	399	FAD	C2B-C3B-C4B	-4.21	94.47	102.61
2	A	399	FAD	O3'-C3'-C2'	-4.15	99.49	108.93
2	B	399	FAD	C5X-N5-C4X	-4.14	111.39	118.09
2	D	399	FAD	C6-C5X-N5	-4.02	111.78	118.44
2	D	399	FAD	O4B-C1B-C2B	-3.95	98.17	106.62
2	A	399	FAD	O4-C4-N3	-3.94	112.71	120.11
2	A	399	FAD	C9A-C5X-N5	3.87	126.56	122.45
2	B	399	FAD	O5B-C5B-C4B	3.85	122.10	108.99
2	B	399	FAD	C4-C4X-N5	-3.85	112.89	118.21
2	D	399	FAD	C4-C4X-N5	-3.76	113.01	118.21
2	A	399	FAD	O2-C2-N1	3.57	127.73	121.80
2	C	399	FAD	O2-C2-N1	3.56	127.71	121.80
2	D	399	FAD	O4B-C4B-C3B	3.43	111.96	105.15
2	A	399	FAD	O4B-C4B-C3B	-3.38	98.44	105.15
2	C	399	FAD	C9A-C5X-N5	3.34	126.00	122.45
2	D	399	FAD	O3P-P-O1P	3.24	120.45	110.70
2	D	399	FAD	C5X-N5-C4X	-3.20	112.91	118.09
2	C	399	FAD	C5X-N5-C4X	-3.18	112.95	118.09
2	D	399	FAD	C4'-C3'-C2'	-3.17	108.30	113.57
2	C	399	FAD	O4-C4-N3	-3.05	114.38	120.11
2	C	399	FAD	O4B-C1B-C2B	-2.97	100.26	106.62
2	D	399	FAD	C4A-N9A-C8A	-2.97	102.62	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	399	FAD	C5X-N5-C4X	-2.95	113.31	118.09
2	D	399	FAD	C3B-C2B-C1B	2.92	106.98	101.46
2	A	399	FAD	C2B-C3B-C4B	-2.87	97.07	102.61
2	B	399	FAD	O4B-C1B-C2B	-2.80	100.62	106.62
2	C	399	FAD	O4B-C1B-N9A	2.63	113.13	108.09
2	D	399	FAD	C4A-N9A-C1B	2.51	132.51	126.63
2	D	399	FAD	C7M-C7-C8	2.48	125.83	120.76
2	A	399	FAD	O4'-C4'-C3'	2.40	114.87	109.25
2	B	399	FAD	C6-C5X-N5	-2.37	114.52	118.44
2	A	399	FAD	O2A-PA-O1A	2.35	123.39	112.44
2	B	399	FAD	O4'-C4'-C5'	-2.34	104.82	109.99
2	C	399	FAD	O4'-C4'-C5'	-2.34	104.82	109.99
2	B	399	FAD	C2B-C3B-C4B	-2.34	98.09	102.61
2	B	399	FAD	C2B-C1B-N9A	-2.34	107.50	113.30
2	C	399	FAD	C4-C4X-N5	-2.34	114.98	118.21
2	D	399	FAD	O4B-C1B-N9A	2.31	112.52	108.09
2	D	399	FAD	O2A-PA-O1A	2.20	122.70	112.44
2	C	399	FAD	PA-O5B-C5B	-2.20	108.72	121.35
2	A	399	FAD	C4'-C3'-C2'	2.19	117.22	113.57
2	A	399	FAD	O4B-C1B-C2B	-2.13	102.06	106.62
2	C	399	FAD	P-O5'-C5'	-2.10	109.31	121.35
2	B	399	FAD	O2P-P-O3P	2.05	112.80	107.27
2	A	399	FAD	C5X-C9A-N10	-2.02	116.14	117.97

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	399	FAD	C5B-O5B-PA-O2A
2	B	399	FAD	C5B-O5B-PA-O2A
2	B	399	FAD	C3'-C4'-C5'-O5'
2	B	399	FAD	O4'-C4'-C5'-O5'
2	C	399	FAD	C5B-O5B-PA-O1A
2	D	399	FAD	C5B-O5B-PA-O3P
2	D	399	FAD	C2'-C3'-C4'-O4'
2	D	399	FAD	O3'-C3'-C4'-O4'
2	D	399	FAD	O3'-C3'-C4'-C5'
2	D	399	FAD	C5'-O5'-P-O1P
2	D	399	FAD	C5'-O5'-P-O3P
2	D	399	FAD	C2'-C3'-C4'-C5'
2	B	399	FAD	O2'-C2'-C3'-O3'
2	C	399	FAD	O3'-C3'-C4'-O4'

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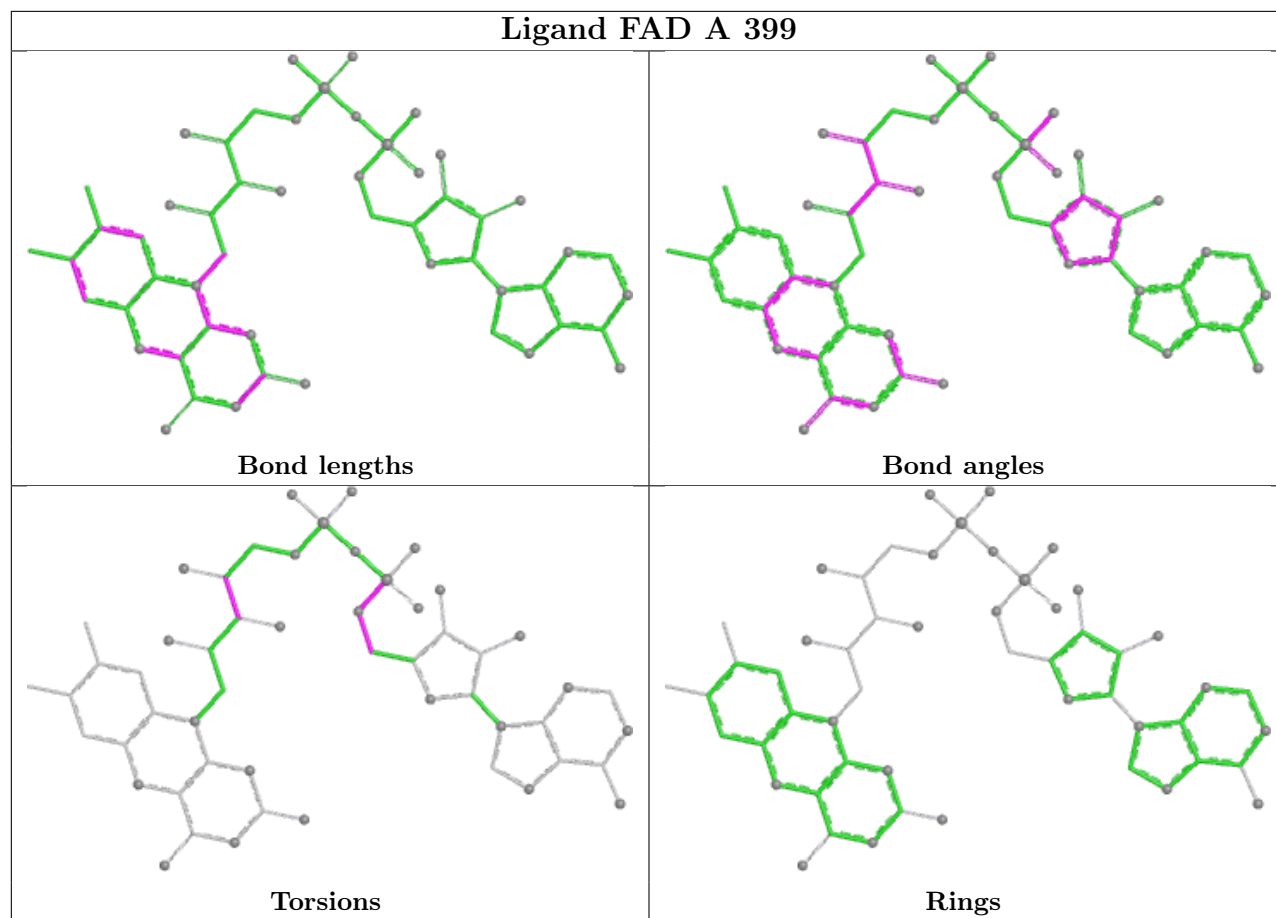
Mol	Chain	Res	Type	Atoms
2	B	399	FAD	O2'-C2'-C3'-C4'
2	B	399	FAD	C1'-C2'-C3'-O3'
2	C	399	FAD	C2'-C3'-C4'-O4'
2	A	399	FAD	C5B-O5B-PA-O1A
2	A	399	FAD	C5B-O5B-PA-O3P
2	B	399	FAD	C5B-O5B-PA-O3P
2	C	399	FAD	C5B-O5B-PA-O2A
2	C	399	FAD	C5B-O5B-PA-O3P
2	D	399	FAD	C5B-O5B-PA-O1A
2	D	399	FAD	C5'-O5'-P-O2P
2	C	399	FAD	PA-O3P-P-O2P
2	C	399	FAD	O3'-C3'-C4'-C5'
2	B	399	FAD	C2'-C3'-C4'-O4'
2	C	399	FAD	PA-O3P-P-O1P
2	A	399	FAD	O3'-C3'-C4'-C5'
2	B	399	FAD	C4'-C5'-O5'-P
2	A	399	FAD	C4B-C5B-O5B-PA

There are no ring outliers.

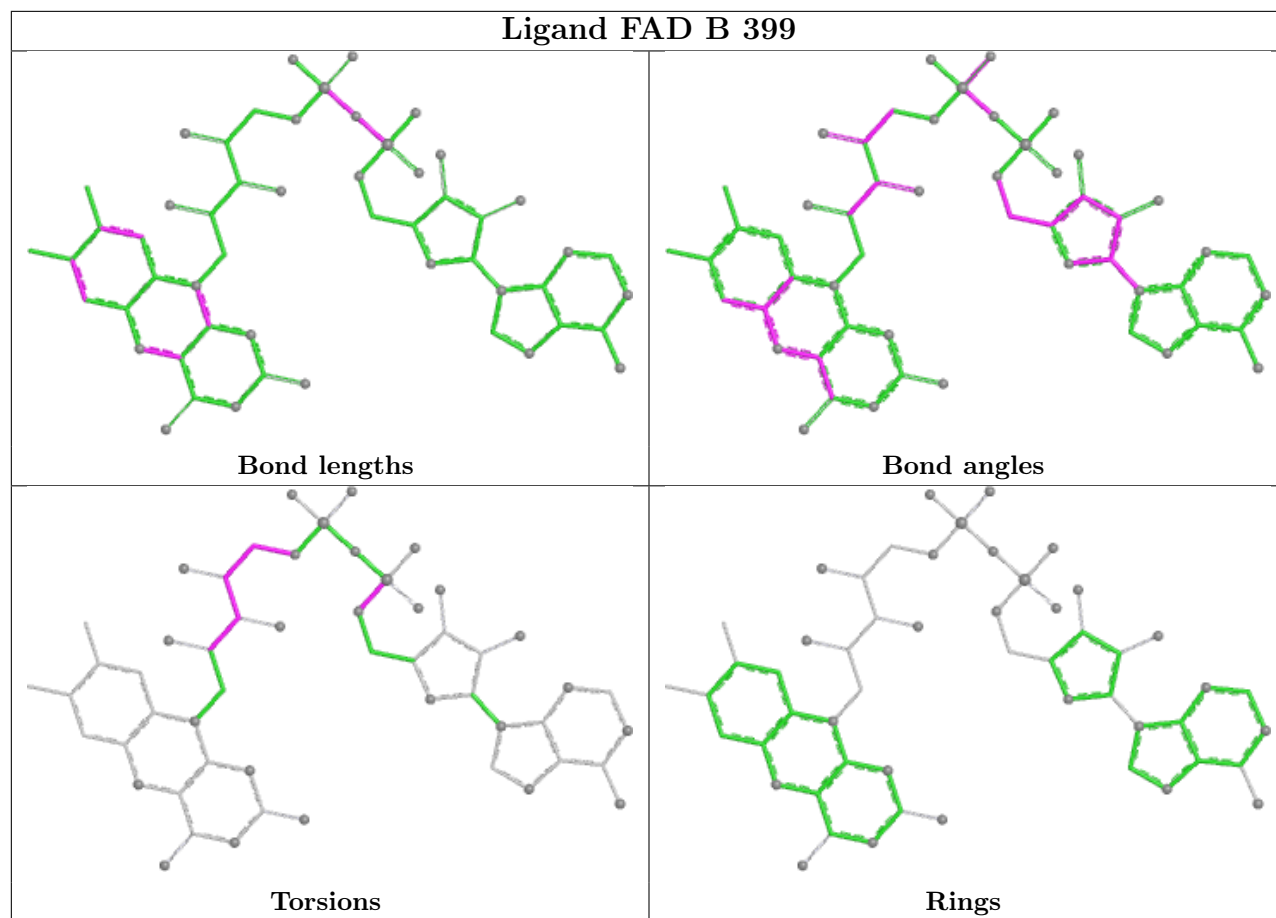
4 monomers are involved in 11 short contacts:

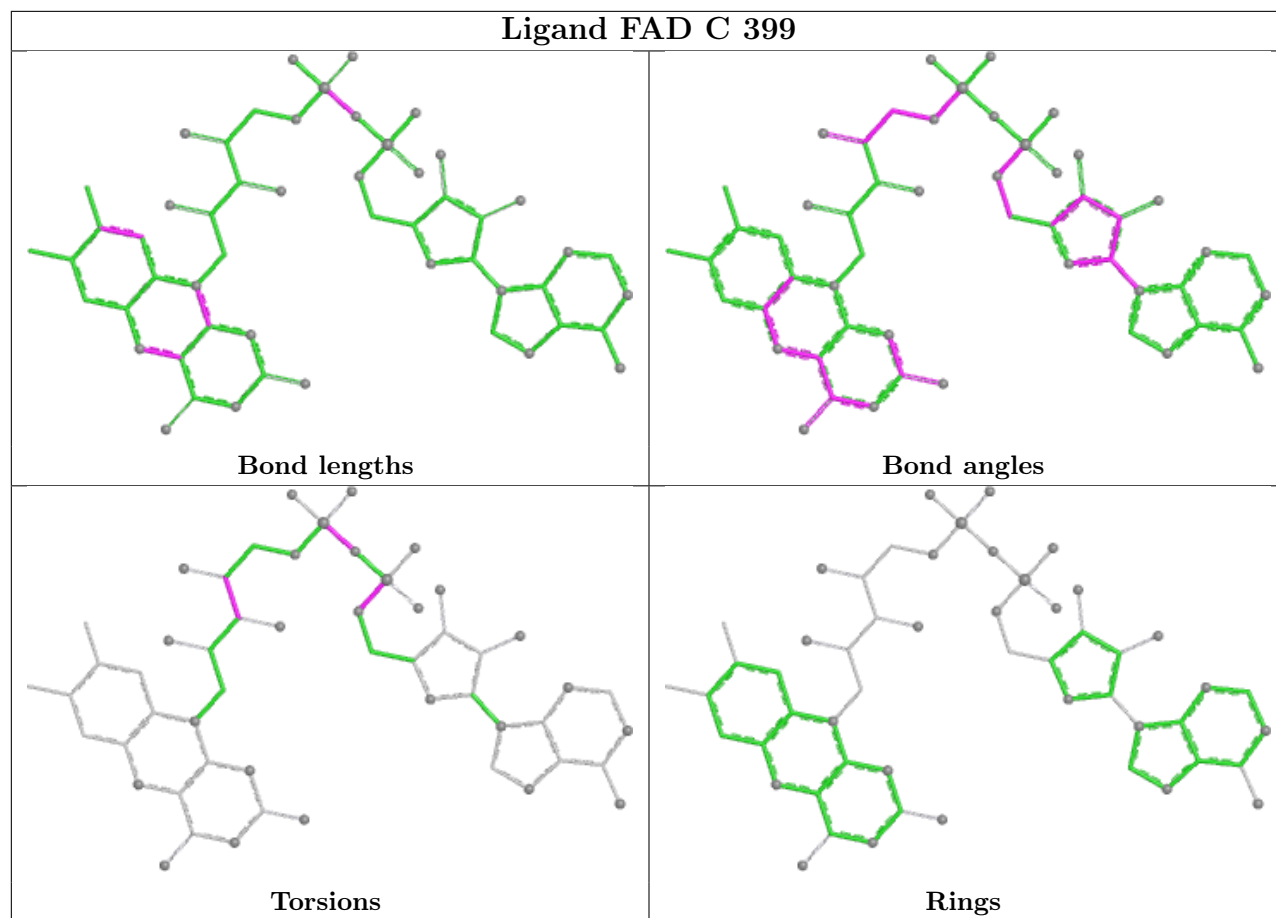
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	399	FAD	5	0
2	B	399	FAD	1	0
2	C	399	FAD	4	0
2	D	399	FAD	1	0

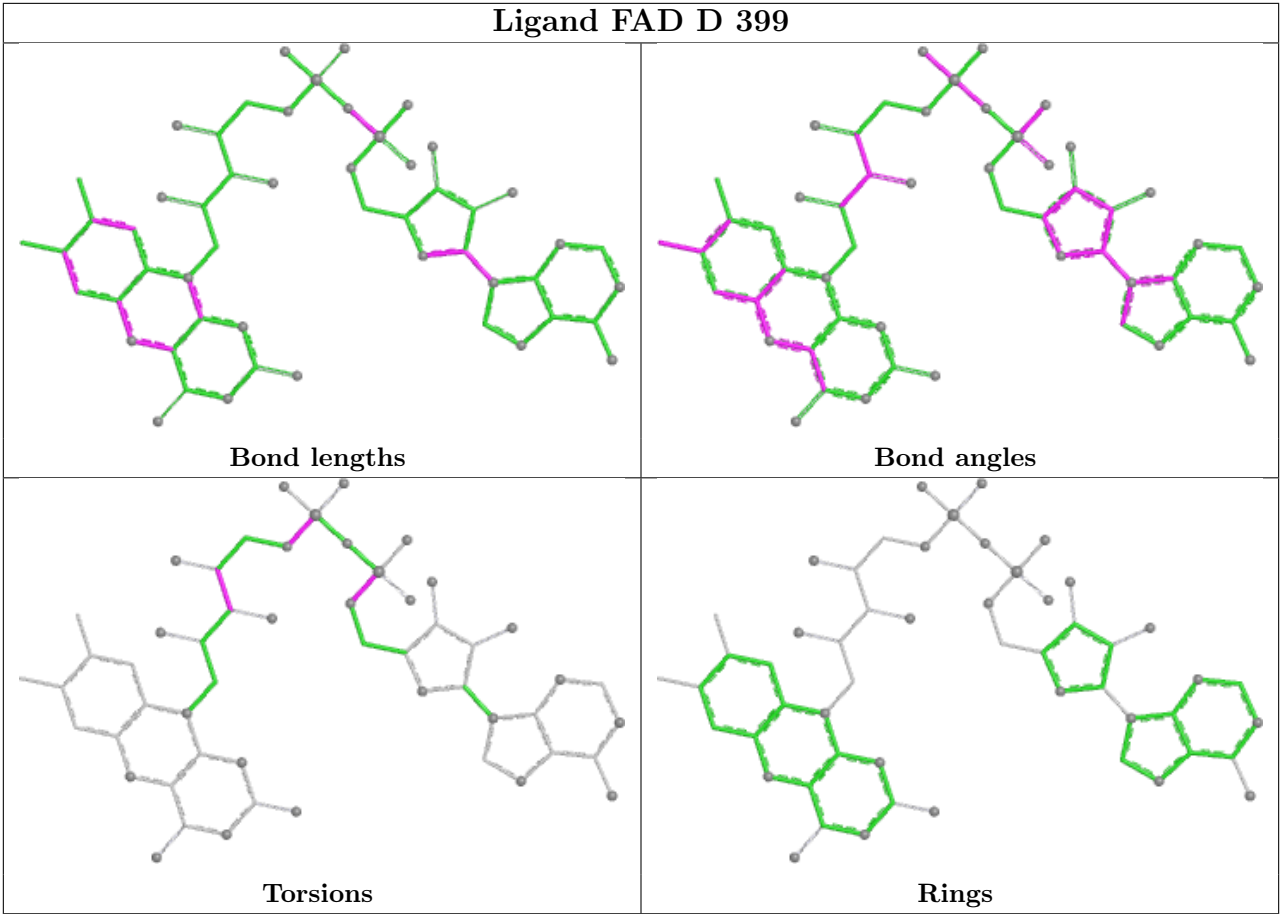
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



Ligand FAD B 399







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1
1	D	1
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	226:VAL	C	227:PHE	N	1.18
1	D	214:ASN	C	215:MET	N	1.14
1	B	324:ARG	C	325:ASN	N	1.00

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.