



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:10 PM UTC

PDB ID : 1EGD / pdb_00001egd
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 : 2.40 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

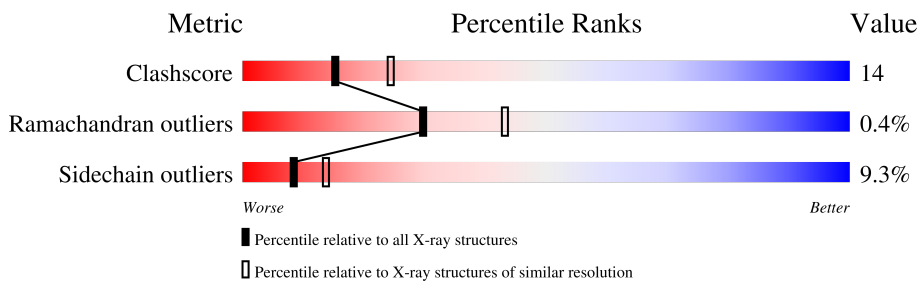
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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

There are 3 unique types of molecules in this entry. The entry contains 12400 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
			2990	1892	515	565	18			
1	B	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	C	387	Total	C	N	O	S	0	0	0
			2990	1892	515	565	18			
1	D	387	Total	C	N	O	S	5	0	0
			2990	1892	515	565	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	255	GLU	THR	engineered mutation	UNP P11310
A	376	GLY	GLU	engineered mutation	UNP P11310
B	255	GLU	THR	engineered mutation	UNP P11310
B	376	GLY	GLU	engineered mutation	UNP P11310
C	255	GLU	THR	engineered mutation	UNP P11310
C	376	GLY	GLU	engineered mutation	UNP P11310
D	255	GLU	THR	engineered mutation	UNP P11310
D	376	GLY	GLU	engineered mutation	UNP P11310

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0
3	B	61	Total O 61 61	0	0
3	C	68	Total O 68 68	0	0
3	D	44	Total O 44 44	0	0

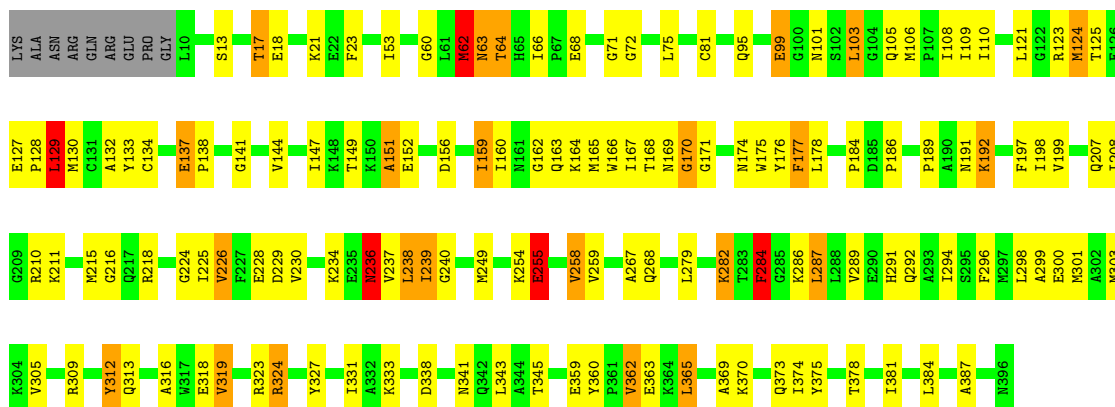
3 Residue-property plots

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.

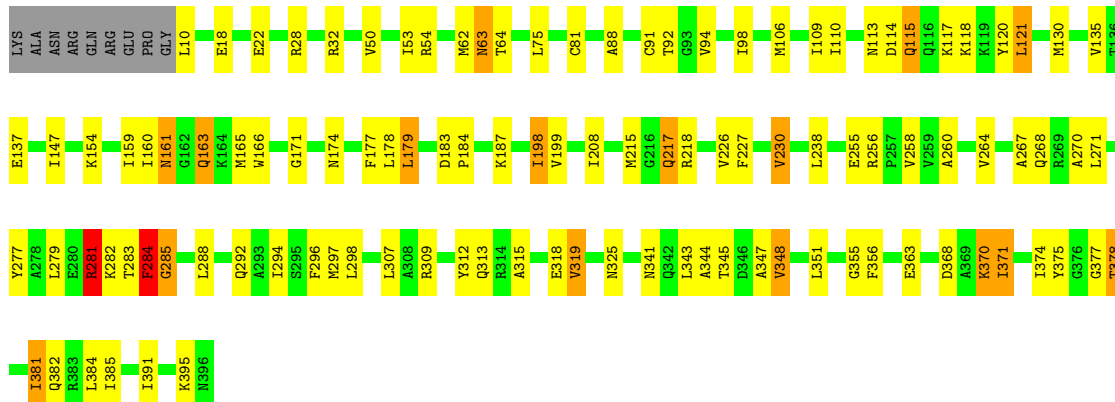
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A: 



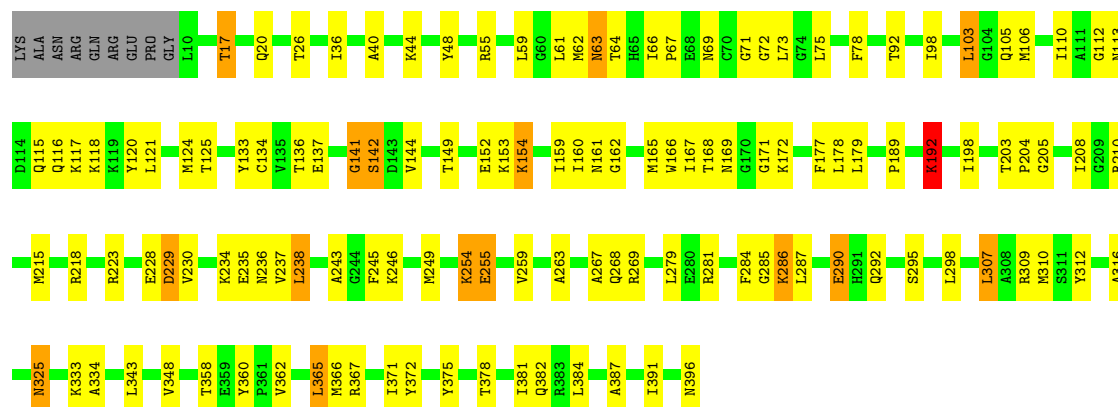
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B: 



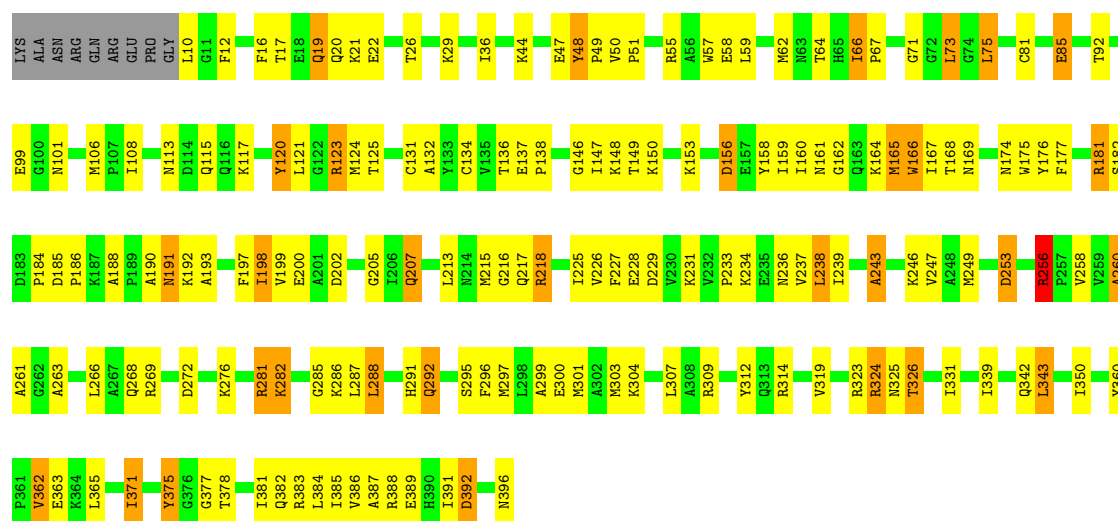
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C: 



● Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D: 55% 35% 8% .



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	170.18Å 170.18Å 150.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.208 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12400	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.22	11/3045 (0.4%)	1.73	28/4102 (0.7%)
1	B	0.66	4/3045 (0.1%)	1.12	14/4102 (0.3%)
1	C	0.63	6/3045 (0.2%)	1.12	20/4102 (0.5%)
1	D	0.93	6/3045 (0.2%)	1.19	25/4102 (0.6%)
All	All	0.89	27/12180 (0.2%)	1.31	87/16408 (0.5%)

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	4
All	All	0	12

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PHE	CD1-CE1	46.89	2.79	1.38
1	D	260	ALA	C-N	30.01	1.72	1.33
1	A	240	GLY	C-N	-22.03	1.03	1.33
1	A	282	LYS	C-N	-12.89	1.15	1.33
1	B	395	LYS	C-N	12.25	1.50	1.33
1	A	226	VAL	C-N	-10.37	1.19	1.33
1	C	281	ARG	C-N	-9.90	1.20	1.33
1	A	236	ASN	C-N	9.67	1.47	1.33
1	D	281	ARG	C-N	-9.59	1.19	1.33
1	D	243	ALA	C-N	-9.04	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	323	ARG	C-N	8.83	1.45	1.33
1	A	129	LEU	N-CA	-8.81	1.35	1.46
1	A	128	PRO	C-N	-8.51	1.21	1.33
1	A	60	GLY	C-N	-7.93	1.23	1.33
1	A	129	LEU	C-N	-7.76	1.22	1.33
1	C	229	ASP	C-N	6.11	1.41	1.33
1	A	239	ILE	N-CA	6.06	1.53	1.46
1	B	284	PHE	C-N	6.00	1.42	1.33
1	A	128	PRO	C-O	5.97	1.31	1.24
1	B	281	ARG	C-N	-5.82	1.26	1.33
1	C	36	ILE	CA-CB	5.81	1.57	1.54
1	C	285	GLY	C-N	5.62	1.41	1.33
1	C	64	THR	C-N	-5.52	1.25	1.33
1	D	166	TRP	NE1-CE2	-5.28	1.31	1.37
1	B	230	VAL	C-N	-5.27	1.25	1.33
1	D	44	LYS	C-N	5.17	1.41	1.33
1	C	205	GLY	N-CA	5.10	1.53	1.45

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PHE	CE1-CZ-CE2	-66.47	0.35	120.00
1	A	284	PHE	CG-CD1-CE1	-35.57	60.24	120.70
1	A	284	PHE	CD1-CE1-CZ	-33.10	60.42	120.00
1	B	395	LYS	O-C-N	17.21	144.33	121.78
1	C	64	THR	O-C-N	-15.90	104.08	122.20
1	A	218	ARG	O-C-N	-14.04	105.79	122.22
1	C	218	ARG	O-C-N	-12.58	107.86	122.20
1	D	218	ARG	O-C-N	-11.72	108.84	122.20
1	B	218	ARG	O-C-N	-10.99	107.97	122.59
1	B	64	THR	O-C-N	-10.45	108.80	122.39
1	A	170	GLY	O-C-N	-10.32	109.28	122.70
1	B	395	LYS	CA-C-N	-9.61	104.40	121.70
1	B	395	LYS	C-N-CA	-9.61	104.40	121.70
1	A	282	LYS	CA-C-N	9.20	138.19	122.37
1	A	282	LYS	C-N-CA	9.20	138.19	122.37
1	C	362	VAL	N-CA-C	8.95	119.51	110.82
1	A	255	GLU	N-CA-CB	-8.92	96.95	110.33
1	B	255	GLU	CA-CB-CG	-8.91	96.28	114.10
1	D	190	ALA	O-C-N	8.85	134.35	122.59
1	B	177	PHE	N-CA-C	-8.56	95.28	109.07
1	A	128	PRO	O-C-N	8.27	133.81	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	360	TYR	CA-C-N	8.11	127.69	118.85
1	A	360	TYR	C-N-CA	8.11	127.69	118.85
1	B	238	LEU	N-CA-C	8.10	119.80	110.97
1	D	191	ASN	O-C-N	8.09	131.41	122.11
1	B	255	GLU	N-CA-CB	8.07	122.40	110.53
1	D	66	ILE	CA-C-N	8.00	128.00	119.76
1	D	66	ILE	C-N-CA	8.00	128.00	119.76
1	A	226	VAL	CA-C-N	7.96	134.11	122.41
1	A	226	VAL	C-N-CA	7.96	134.11	122.41
1	A	282	LYS	O-C-N	-7.79	113.31	123.21
1	A	226	VAL	O-C-N	-7.73	114.06	123.10
1	D	243	ALA	CA-C-N	7.71	128.34	119.94
1	D	243	ALA	C-N-CA	7.71	128.34	119.94
1	D	362	VAL	N-CA-C	7.69	119.39	110.62
1	C	177	PHE	N-CA-C	-7.65	96.75	109.07
1	C	228	GLU	O-C-N	7.35	131.66	122.84
1	D	190	ALA	CA-C-N	7.17	131.57	120.82
1	D	190	ALA	C-N-CA	7.17	131.57	120.82
1	C	281	ARG	CA-C-N	7.15	132.86	122.77
1	C	281	ARG	C-N-CA	7.15	132.86	122.77
1	A	63	ASN	O-C-N	6.94	131.50	122.20
1	D	285	GLY	O-C-N	-6.89	116.03	122.50
1	A	177	PHE	N-CA-C	-6.88	98.02	108.96
1	C	238	LEU	N-CA-C	6.81	118.40	110.97
1	D	177	PHE	N-CA-C	-6.80	97.33	108.41
1	B	370	LYS	N-CA-C	6.76	119.51	111.33
1	D	360	TYR	CA-C-N	6.73	126.99	119.32
1	D	360	TYR	C-N-CA	6.73	126.99	119.32
1	A	238	LEU	O-C-N	-6.71	113.67	122.59
1	C	360	TYR	CA-C-N	6.69	126.39	119.56
1	C	360	TYR	C-N-CA	6.69	126.39	119.56
1	D	326	THR	O-C-N	-6.53	113.90	122.59
1	C	198	ILE	N-CA-C	-6.15	98.89	107.80
1	C	255	GLU	CA-CB-CG	6.06	126.22	114.10
1	A	64	THR	O-C-N	-5.92	114.72	122.59
1	D	59	LEU	CA-C-N	5.87	131.09	122.10
1	D	59	LEU	C-N-CA	5.87	131.09	122.10
1	B	285	GLY	N-CA-C	-5.77	108.09	115.42
1	C	236	ASN	N-CA-C	5.77	120.05	113.19
1	C	218	ARG	NE-CZ-NH2	5.75	124.38	119.20
1	A	62	MET	N-CA-C	5.68	120.22	113.12
1	D	331	ILE	N-CA-C	-5.62	105.04	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	THR	N-CA-C	-5.53	103.39	110.53
1	B	174	ASN	N-CA-C	-5.46	105.74	112.90
1	D	205	GLY	O-C-N	5.41	127.04	122.71
1	C	281	ARG	O-C-N	-5.40	116.49	122.86
1	A	198	ILE	N-CA-C	-5.38	100.38	108.12
1	A	151	ALA	N-CA-C	-5.37	99.53	108.34
1	A	259	VAL	N-CA-C	-5.35	105.17	111.00
1	A	362	VAL	N-CA-C	5.33	116.69	110.62
1	D	292	GLN	N-CA-C	5.29	117.73	111.33
1	C	285	GLY	N-CA-C	-5.25	108.39	115.21
1	B	218	ARG	NE-CZ-NH2	5.24	123.92	119.20
1	C	17	THR	N-CA-C	-5.24	102.76	110.52
1	D	160	ILE	O-C-N	5.24	128.91	123.26
1	A	218	ARG	NE-CZ-NH2	5.22	123.90	119.20
1	A	369	ALA	N-CA-C	5.21	118.42	111.75
1	B	63	ASN	O-C-N	-5.20	116.11	122.55
1	C	120	TYR	N-CA-C	5.16	118.73	112.23
1	D	202	ASP	N-CA-C	5.15	117.64	111.71
1	A	287	LEU	N-CA-C	-5.09	102.94	110.48
1	D	120	TYR	N-CA-C	5.06	119.48	112.45
1	C	124	MET	N-CA-C	-5.04	106.39	112.54
1	C	230	VAL	O-C-N	5.04	129.08	122.94
1	D	324	ARG	NE-CZ-NH2	5.02	123.72	119.20
1	D	123	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	129	LEU	Mainchain
1	A	170	GLY	Mainchain
1	A	284	PHE	Mainchain
1	B	284	PHE	Mainchain
1	B	63	ASN	Mainchain
1	C	229	ASP	Mainchain
1	C	284	PHE	Mainchain
1	C	63	ASN	Mainchain
1	D	181	ARG	Sidechain
1	D	217	GLN	Mainchain
1	D	239	ILE	Mainchain
1	D	256	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	2990	0	2975	88	0
1	B	2990	0	2978	67	0
1	C	2990	0	2978	84	0
1	D	2990	0	2977	117	0
2	A	53	0	31	1	0
2	B	53	0	31	1	0
2	C	53	0	31	1	0
2	D	53	0	31	1	0
3	A	55	0	0	0	0
3	B	61	0	0	2	0
3	C	68	0	0	3	0
3	D	44	0	0	2	0
All	All	12400	0	12032	330	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 14.

All (330) 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:260:ALA:C	1:D:261:ALA:N	1.72	1.47
1:D:256:ARG:HG3	1:D:256:ARG:HH11	1.20	1.01
1:C:103:LEU:O	1:C:103:LEU:HD22	1.63	0.99
1:A:189:PRO:HG2	1:A:192:LYS:HG2	1.46	0.95
1:A:284:PHE:CD1	1:A:284:PHE:CZ	2.43	0.94
1:B:374:ILE:HA	1:B:378:THR:HG22	1.50	0.90
1:A:106:MET:HE2	1:A:254:LYS:HG2	1.52	0.89
1:A:363:GLU:HG3	1:B:215:MET:HB2	1.56	0.88
1:C:103:LEU:HD13	1:C:133:TYR:CB	2.08	0.83
1:B:268:GLN:HE21	1:B:309:ARG:HH22	1.29	0.81
1:D:156:ASP:HA	1:D:234:LYS:HD3	1.62	0.80
1:D:268:GLN:HE21	1:D:309:ARG:HH22	1.30	0.79
1:B:62:MET:HG3	1:B:98:ILE:HG23	1.64	0.79
1:D:256:ARG:HD2	3:D:2124:HOH:O	1.83	0.78
1:C:103:LEU:HD13	1:C:133:TYR:CG	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:HB2	1:A:159:ILE:HG23	1.68	0.75
1:D:256:ARG:HG3	1:D:256:ARG:NH1	1.97	0.75
1:B:154:LYS:HD2	1:B:159:ILE:HD12	1.68	0.75
1:A:168:THR:O	1:A:169:ASN:HB2	1.85	0.75
1:A:17:THR:HG22	1:D:10:LEU:HG	1.70	0.73
1:D:192:LYS:HD2	1:D:192:LYS:O	1.90	0.71
1:D:256:ARG:HH11	1:D:256:ARG:CG	2.01	0.71
1:C:171:GLY:HA2	1:C:208:ILE:HD13	1.72	0.71
1:B:294:ILE:HD13	1:B:297:MET:CE	2.22	0.70
1:D:99:GLU:OE2	1:D:258:VAL:HG11	1.92	0.70
1:B:294:ILE:HD13	1:B:297:MET:HE3	1.73	0.69
1:D:121:LEU:O	1:D:124:MET:HB2	1.93	0.69
1:B:160:ILE:HG21	1:B:178:LEU:HD21	1.74	0.68
1:C:103:LEU:HD22	1:C:103:LEU:C	2.18	0.68
1:B:374:ILE:HA	1:B:378:THR:CG2	2.24	0.68
1:B:163:GLN:HG2	1:B:226:VAL:HG22	1.76	0.68
1:A:123:ARG:HB3	1:A:129:LEU:HD13	1.77	0.67
1:B:18:GLU:O	1:B:22:GLU:HG2	1.95	0.67
1:C:215:MET:HB2	1:D:363:GLU:HG3	1.75	0.67
1:C:62:MET:SD	1:C:98:ILE:HG23	2.36	0.66
1:D:153:LYS:HE3	1:D:234:LYS:HD2	1.77	0.66
1:C:160:ILE:HG21	1:C:178:LEU:HD21	1.78	0.66
1:B:106:MET:HE2	1:B:110:ILE:HG23	1.78	0.66
1:C:71:GLY:HA3	1:C:125:THR:HG21	1.78	0.66
1:D:256:ARG:CD	3:D:2124:HOH:O	2.41	0.66
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.60	0.65
1:D:123:ARG:HH11	1:D:174:ASN:HD21	1.44	0.64
1:D:134:CYS:SG	1:D:225:ILE:HD12	2.37	0.64
1:C:153:LYS:O	1:C:154:LYS:HE3	1.97	0.64
1:A:106:MET:O	1:A:110:ILE:HG12	1.97	0.63
1:C:106:MET:SD	1:C:254:LYS:HE3	2.39	0.63
1:D:120:TYR:O	1:D:124:MET:HG2	1.99	0.63
1:D:134:CYS:HA	1:D:167:ILE:HD12	1.82	0.62
1:A:309:ARG:O	1:A:313:GLN:HG3	1.99	0.62
1:D:300:GLU:O	1:D:304:LYS:HG3	1.99	0.62
1:A:68:GLU:HA	1:A:72:GLY:O	1.99	0.62
1:A:71:GLY:HA3	1:A:125:THR:HG21	1.81	0.62
1:D:149:THR:HG23	1:D:162:GLY:HA3	1.81	0.61
1:D:19:GLN:CD	1:D:19:GLN:H	2.08	0.61
1:D:123:ARG:HH11	1:D:174:ASN:ND2	1.98	0.61
1:A:105:GLN:O	1:A:109:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:ALA:HB1	1:B:92:THR:HG22	1.83	0.60
1:D:16:PHE:O	1:D:21:LYS:HE3	2.01	0.60
1:A:228:GLU:O	1:A:229:ASP:HB2	2.01	0.60
1:B:117:LYS:O	1:B:121:LEU:HB2	2.02	0.60
1:B:292:GLN:HB3	1:D:292:GLN:HB2	1.84	0.60
1:D:66:ILE:HG12	1:D:121:LEU:HD12	1.83	0.59
1:C:103:LEU:O	1:C:103:LEU:CD2	2.46	0.59
1:D:213:LEU:N	1:D:213:LEU:HD22	2.18	0.59
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.83	0.58
1:D:138:PRO:HD3	1:D:165:MET:HB2	1.84	0.58
1:A:149:THR:HG23	1:A:162:GLY:HA3	1.84	0.58
1:B:377:GLY:HA2	3:B:2048:HOH:O	2.02	0.58
1:A:370:LYS:NZ	1:B:345:THR:HG22	2.18	0.58
1:D:282:LYS:HE3	1:D:287:LEU:HD12	1.86	0.58
1:C:103:LEU:HD13	1:C:133:TYR:HB2	1.85	0.58
1:B:53:ILE:HG21	1:B:130:MET:HE1	1.86	0.58
1:D:150:LYS:NZ	1:D:184:PRO:HG3	2.18	0.58
1:C:106:MET:O	1:C:110:ILE:HG12	2.04	0.57
1:C:171:GLY:N	1:C:223:ARG:HD2	2.19	0.57
1:C:367:ARG:HG3	1:D:215:MET:HE2	1.86	0.57
1:D:268:GLN:NE2	1:D:309:ARG:HH22	2.01	0.57
1:C:113:ASN:H	1:C:116:GLN:HE21	1.50	0.57
1:C:259:VAL:HG23	1:C:333:LYS:HD3	1.86	0.57
1:A:207:GLN:NE2	1:A:228:GLU:HB2	2.20	0.57
1:C:73:LEU:HB3	1:C:75:LEU:HD13	1.87	0.57
1:C:325:ASN:H	1:C:325:ASN:HD22	1.53	0.57
1:C:366:MET:HB3	1:D:215:MET:HE1	1.86	0.57
1:D:182:SER:O	1:D:184:PRO:HD3	2.04	0.57
1:C:154:LYS:HE3	1:C:154:LYS:HA	1.87	0.56
1:C:189:PRO:HG2	1:C:192:LYS:HG2	1.86	0.56
1:C:268:GLN:HE21	1:C:309:ARG:HH22	1.53	0.56
1:D:233:PRO:HD2	1:D:236:ASN:HD22	1.69	0.56
1:D:153:LYS:HB2	1:D:158:TYR:CE2	2.41	0.56
1:D:256:ARG:NH1	1:D:256:ARG:CG	2.63	0.56
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.70	0.56
1:C:103:LEU:C	1:C:103:LEU:CD2	2.78	0.56
1:A:374:ILE:HA	1:A:378:THR:HG22	1.88	0.55
1:D:17:THR:H	1:D:20:GLN:HE21	1.53	0.55
1:A:138:PRO:HD3	1:A:165:MET:HB2	1.88	0.55
1:A:177:PHE:HE1	1:A:238:LEU:HD12	1.70	0.55
1:B:341:ASN:HD21	1:B:370:LYS:HA	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:GLY:O	1:D:148:LYS:HD3	2.06	0.55
1:A:255:GLU:O	1:A:258:VAL:HG13	2.07	0.55
1:A:215:MET:HB2	1:B:363:GLU:HG3	1.89	0.54
1:D:175:TRP:HA	1:D:200:GLU:HA	1.90	0.54
1:B:135:VAL:HG22	1:B:179:LEU:HB2	1.90	0.54
1:D:159:ILE:HD13	1:D:231:LYS:HE3	1.88	0.54
1:D:297:MET:O	1:D:301:MET:HG3	2.07	0.54
1:B:270:ALA:HB1	1:B:347:ALA:HB2	1.89	0.54
1:A:384:LEU:HD21	1:D:292:GLN:HE21	1.73	0.54
1:A:216:GLY:HA3	1:B:356:PHE:HZ	1.72	0.54
1:B:113:ASN:OD1	1:B:115:GLN:HG2	2.08	0.54
1:C:26:THR:HG22	1:C:61:LEU:HD11	1.89	0.54
1:C:234:LYS:O	1:C:237:VAL:HG22	2.08	0.54
1:B:114:ASP:O	1:B:118:LYS:HB2	2.08	0.53
1:C:243:ALA:O	1:C:246:LYS:HG3	2.08	0.53
1:A:282:LYS:HG3	1:A:287:LEU:HD23	1.91	0.53
1:C:66:ILE:O	1:C:72:GLY:HA3	2.08	0.53
1:D:123:ARG:NH1	1:D:174:ASN:HD21	2.07	0.53
1:A:216:GLY:HA3	1:B:356:PHE:CZ	2.44	0.53
1:D:17:THR:H	1:D:20:GLN:NE2	2.07	0.53
1:D:286:LYS:HG3	1:D:291:HIS:CE1	2.43	0.53
1:A:316:ALA:O	1:A:319:VAL:HG12	2.09	0.52
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.91	0.52
1:A:387:ALA:HB2	1:D:299:ALA:HB2	1.91	0.52
1:A:292:GLN:HE21	1:D:384:LEU:HD21	1.74	0.52
1:C:235:GLU:HG3	3:C:2227:HOH:O	2.09	0.52
1:A:151:ALA:HA	1:A:160:ILE:HD13	1.92	0.52
1:B:319:VAL:HG22	1:B:325:ASN:ND2	2.25	0.52
1:D:215:MET:HG2	1:D:215:MET:O	2.08	0.52
1:C:103:LEU:CD1	1:C:133:TYR:CG	2.92	0.51
1:A:255:GLU:OE1	1:A:255:GLU:HA	2.10	0.51
1:C:171:GLY:H	1:C:223:ARG:HD2	1.75	0.51
1:D:137:GLU:HB3	1:D:138:PRO:HD2	1.93	0.51
1:C:215:MET:HB2	1:D:363:GLU:CG	2.39	0.51
1:C:286:LYS:HD3	1:C:290:GLU:HB3	1.93	0.51
1:D:134:CYS:HB3	1:D:164:LYS:HG3	1.92	0.51
1:B:282:LYS:HD2	1:B:285:GLY:O	2.11	0.51
1:A:165:MET:HG3	1:A:166:TRP:CD1	2.46	0.51
1:B:91:CYS:SG	1:B:94:VAL:HG23	2.51	0.51
1:B:106:MET:CE	1:B:110:ILE:HG23	2.41	0.51
1:C:141:GLY:HA3	2:C:399:FAD:O2P	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:THR:HB	1:D:75:LEU:HB2	1.93	0.50
1:C:286:LYS:NZ	1:C:286:LYS:HB3	2.26	0.50
1:A:124:MET:SD	1:A:124:MET:N	2.83	0.50
1:D:73:LEU:HB3	1:D:75:LEU:HD22	1.94	0.50
1:D:243:ALA:O	1:D:247:VAL:HG23	2.12	0.49
1:A:132:ALA:HB3	1:A:176:TYR:CD1	2.45	0.49
1:C:144:VAL:HG23	1:C:245:PHE:CE1	2.47	0.49
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.47	0.49
1:D:161:ASN:HA	1:D:227:PHE:O	2.12	0.49
1:A:123:ARG:HH11	1:A:174:ASN:HD21	1.60	0.49
1:B:319:VAL:HG22	1:B:325:ASN:CG	2.37	0.49
1:D:117:LYS:HA	1:D:121:LEU:HD23	1.94	0.48
1:A:324:ARG:HH11	1:A:324:ARG:HB3	1.78	0.48
1:C:17:THR:OG1	1:C:20:GLN:HG3	2.13	0.48
1:C:63:ASN:ND2	1:C:105:GLN:HE22	2.10	0.48
2:A:399:FAD:H1B	1:B:294:ILE:HD11	1.95	0.48
1:B:294:ILE:HD13	1:B:297:MET:HE1	1.94	0.48
1:C:40:ALA:O	1:C:44:LYS:HG3	2.13	0.48
1:D:175:TRP:CE3	1:D:198:ILE:HD13	2.49	0.48
1:A:338:ASP:HA	1:A:373:GLN:HE21	1.77	0.48
1:B:318:GLU:HB3	1:B:325:ASN:HB3	1.94	0.48
1:A:66:ILE:HD13	1:A:121:LEU:O	2.13	0.48
1:B:355:GLY:O	1:B:363:GLU:HB2	2.13	0.48
1:C:171:GLY:HA3	1:C:208:ILE:HG21	1.95	0.48
1:D:371:ILE:HD13	1:D:375:TYR:CZ	2.48	0.48
1:C:325:ASN:HD22	1:C:325:ASN:N	2.12	0.48
1:D:153:LYS:CE	1:D:234:LYS:HD2	2.42	0.48
1:D:106:MET:HA	1:D:106:MET:HE3	1.96	0.48
1:A:171:GLY:HA2	1:A:208:ILE:HG21	1.95	0.47
1:B:294:ILE:O	1:B:298:LEU:HG	2.14	0.47
1:C:171:GLY:HA3	1:C:223:ARG:HD2	1.96	0.47
1:D:197:PHE:CE2	1:D:237:VAL:HG22	2.48	0.47
1:D:216:GLY:C	1:D:218:ARG:N	2.72	0.47
1:D:339:ILE:O	1:D:343:LEU:HD23	2.14	0.47
1:A:171:GLY:HA2	1:A:208:ILE:HD13	1.95	0.47
1:C:117:LYS:O	1:C:121:LEU:HB2	2.14	0.47
1:A:318:GLU:HG3	1:A:323:ARG:HG3	1.96	0.47
1:B:120:TYR:CE1	1:B:198:ILE:HD11	2.49	0.47
1:D:150:LYS:HZ2	1:D:184:PRO:HG3	1.78	0.47
1:A:95:GLN:O	1:A:99:GLU:HB2	2.14	0.47
1:A:296:PHE:O	1:A:300:GLU:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:TYR:CZ	1:C:172:LYS:HG2	2.48	0.47
1:A:370:LYS:HZ3	1:B:345:THR:HG22	1.78	0.47
1:A:279:LEU:HD21	1:D:391:ILE:HG23	1.97	0.47
1:A:289:VAL:HG13	1:D:391:ILE:HD13	1.96	0.47
1:A:327:TYR:O	1:A:331:ILE:HG13	2.15	0.47
1:B:309:ARG:O	1:B:313:GLN:HG3	2.14	0.47
1:B:344:ALA:O	1:B:348:VAL:HG13	2.15	0.47
1:A:174:ASN:HD22	1:A:175:TRP:HD1	1.63	0.47
1:D:303:MET:O	1:D:307:LEU:HD23	2.14	0.47
1:A:197:PHE:CE1	1:A:237:VAL:HG22	2.50	0.47
1:C:269:ARG:HG3	1:C:365:LEU:HD21	1.98	0.46
1:D:260:ALA:O	1:D:263:ALA:HB3	2.15	0.46
1:D:304:LYS:HE2	1:D:342:GLN:OE1	2.15	0.46
1:A:53:ILE:HD13	1:A:130:MET:HE2	1.96	0.46
1:A:176:TYR:HB2	1:A:199:VAL:HG22	1.97	0.46
1:A:234:LYS:O	1:A:237:VAL:HG23	2.16	0.46
1:D:132:ALA:HB3	1:D:176:TYR:HD1	1.80	0.46
1:D:181:ARG:NH1	1:D:188:ALA:HB3	2.30	0.46
1:C:154:LYS:HE3	1:C:154:LYS:CA	2.44	0.46
1:A:108:ILE:HD12	1:A:175:TRP:CH2	2.50	0.46
1:D:272:ASP:O	1:D:276:LYS:HG3	2.15	0.46
1:B:161:ASN:HA	1:B:227:PHE:O	2.16	0.46
1:C:267:ALA:HB1	1:C:343:LEU:HD22	1.96	0.46
1:A:207:GLN:HB2	1:A:226:VAL:HB	1.97	0.46
1:C:17:THR:H	1:C:20:GLN:HE21	1.63	0.46
1:C:189:PRO:HG2	1:C:192:LYS:CG	2.46	0.46
1:A:189:PRO:HB2	1:A:191:ASN:OD1	2.14	0.46
1:D:19:GLN:O	1:D:22:GLU:HB2	2.15	0.46
1:B:381:ILE:O	1:B:385:ILE:HG13	2.15	0.45
1:C:171:GLY:CA	1:C:223:ARG:HD2	2.46	0.45
1:A:103:LEU:HD13	1:A:133:TYR:CB	2.46	0.45
1:A:312:TYR:C	1:A:312:TYR:CD1	2.94	0.45
1:B:277:TYR:CE2	1:B:281:ARG:HG3	2.51	0.45
1:D:382:GLN:O	1:D:386:VAL:HG23	2.16	0.45
1:B:283:THR:O	1:B:284:PHE:C	2.60	0.45
1:C:168:THR:O	1:C:169:ASN:HB2	2.16	0.45
1:D:169:ASN:N	1:D:169:ASN:HD22	2.15	0.45
1:A:17:THR:O	1:A:21:LYS:HG3	2.16	0.45
1:A:294:ILE:HD11	2:B:399:FAD:H1B	1.99	0.45
1:C:67:PRO:HD2	1:C:121:LEU:HD23	1.98	0.45
1:B:384:LEU:HD21	1:C:292:GLN:HE21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:GLN:HG3	1:D:226:VAL:HB	1.99	0.45
1:D:238:LEU:HD13	1:D:238:LEU:HA	1.78	0.45
1:D:296:PHE:O	1:D:300:GLU:HG3	2.17	0.45
1:B:315:ALA:O	1:B:319:VAL:HG23	2.17	0.45
1:C:62:MET:HG3	3:C:2021:HOH:O	2.16	0.45
1:C:154:LYS:HD2	1:C:159:ILE:HD11	1.97	0.45
1:D:108:ILE:HG22	1:D:121:LEU:HD21	1.99	0.45
1:D:385:ILE:O	1:D:389:GLU:HG2	2.15	0.45
1:A:224:GLY:C	1:A:225:ILE:HG13	2.41	0.44
1:C:268:GLN:NE2	1:C:309:ARG:HH22	2.14	0.44
1:A:299:ALA:HB2	1:D:387:ALA:HB2	1.99	0.44
1:C:136:THR:HG22	1:C:137:GLU:N	2.33	0.44
1:C:387:ALA:O	1:C:391:ILE:HG12	2.17	0.44
1:C:312:TYR:CD1	1:C:312:TYR:C	2.95	0.44
1:D:19:GLN:CD	1:D:19:GLN:N	2.75	0.44
1:B:106:MET:HE3	1:B:109:ILE:HB	1.99	0.44
1:D:48:TYR:CD1	1:D:49:PRO:HD2	2.53	0.44
1:D:66:ILE:HA	1:D:67:PRO:HD3	1.73	0.44
1:D:137:GLU:OE2	1:D:147:ILE:HG23	2.18	0.44
1:A:177:PHE:CE1	1:A:238:LEU:HD12	2.52	0.44
1:A:184:PRO:O	1:A:186:PRO:HD3	2.18	0.44
1:A:299:ALA:O	1:A:303:MET:HG3	2.18	0.44
1:D:36:ILE:HG12	1:D:269:ARG:HH21	1.81	0.44
1:A:210:ARG:HG3	1:A:211:LYS:N	2.32	0.44
1:C:144:VAL:HG21	1:C:249:MET:HE3	1.99	0.44
1:B:296:PHE:HE1	1:C:384:LEU:HD13	1.83	0.43
1:D:99:GLU:OE1	1:D:99:GLU:HA	2.18	0.43
1:C:103:LEU:HD13	1:C:133:TYR:HB3	1.96	0.43
1:D:168:THR:O	1:D:169:ASN:HB2	2.19	0.43
1:D:81:CYS:HB3	1:D:312:TYR:CE1	2.54	0.43
1:D:136:THR:HG21	2:D:399:FAD:H1'1	1.99	0.43
1:D:159:ILE:HD11	1:D:229:ASP:HA	1.99	0.43
1:A:137:GLU:HB3	1:A:163:GLN:O	2.18	0.43
1:C:203:THR:CG2	1:C:204:PRO:HD2	2.48	0.43
1:D:228:GLU:O	1:D:229:ASP:HB2	2.18	0.43
1:A:289:VAL:CG1	1:D:391:ILE:HD13	2.49	0.43
1:B:260:ALA:O	1:B:264:VAL:HG23	2.18	0.43
1:C:112:GLY:O	1:C:117:LYS:HE3	2.17	0.43
1:D:85:GLU:OE2	1:D:309:ARG:HD3	2.18	0.43
1:D:388:ARG:O	1:D:392:ASP:HB2	2.18	0.43
1:A:282:LYS:HA	1:A:286:LYS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:50:VAL:HB	1:D:51:PRO:HD3	2.00	0.43
1:A:106:MET:CE	1:A:254:LYS:HG2	2.37	0.43
1:A:215:MET:HB2	1:B:363:GLU:CG	2.48	0.43
1:B:137:GLU:OE2	1:B:147:ILE:HB	2.18	0.43
1:B:227:PHE:HD2	1:B:230:VAL:HG21	1.82	0.43
1:D:213:LEU:N	1:D:213:LEU:CD2	2.80	0.43
1:C:263:ALA:HB2	1:C:372:TYR:CD1	2.54	0.43
1:A:255:GLU:OE1	1:A:255:GLU:CA	2.66	0.43
1:C:334:ALA:HA	3:C:2051:HOH:O	2.19	0.43
1:A:301:MET:O	1:A:305:VAL:HG23	2.18	0.42
1:C:165:MET:HG3	1:C:166:TRP:CD1	2.54	0.42
1:A:341:ASN:O	1:A:345:THR:HG22	2.18	0.42
1:C:55:ARG:O	1:C:59:LEU:HG	2.19	0.42
1:C:78:PHE:HA	1:C:316:ALA:HB1	2.00	0.42
1:D:57:TRP:HD1	1:D:62:MET:HE2	1.84	0.42
1:D:185:ASP:HA	1:D:186:PRO:HD2	1.82	0.42
1:D:249:MET:O	1:D:253:ASP:HB2	2.20	0.42
1:A:134:CYS:HB3	1:A:164:LYS:HG3	2.00	0.42
1:A:236:ASN:HD22	1:A:236:ASN:HA	1.65	0.42
1:C:378:THR:O	1:C:382:GLN:HG2	2.19	0.42
1:B:171:GLY:HA2	1:B:208:ILE:HD13	2.02	0.42
1:D:260:ALA:CA	1:D:261:ALA:N	2.72	0.42
1:C:103:LEU:HD23	1:C:103:LEU:HA	1.60	0.42
1:A:267:ALA:HB1	1:A:343:LEU:HD22	2.00	0.42
1:D:281:ARG:HB3	1:D:288:LEU:HD22	2.00	0.42
1:A:62:MET:HE2	1:A:63:ASN:HD21	1.85	0.42
1:A:296:PHE:HE1	1:D:384:LEU:CD2	2.32	0.42
1:D:71:GLY:HA3	1:D:125:THR:HG21	2.02	0.42
1:B:28:ARG:HG3	1:B:32:ARG:NH1	2.34	0.42
1:C:103:LEU:HD11	1:C:133:TYR:CD2	2.55	0.42
1:C:115:GLN:OE1	1:C:115:GLN:N	2.53	0.42
1:B:147:ILE:HD11	1:B:179:LEU:HD13	2.00	0.42
1:B:267:ALA:HB1	1:B:343:LEU:HD22	2.00	0.42
1:C:149:THR:HG23	1:C:162:GLY:HA3	2.02	0.42
1:C:154:LYS:HD2	1:C:159:ILE:CD1	2.50	0.42
1:D:29:LYS:HD2	1:D:29:LYS:C	2.45	0.42
1:A:286:LYS:HB2	1:A:291:HIS:CE1	2.55	0.41
1:B:268:GLN:NE2	1:B:309:ARG:HH22	2.06	0.41
1:C:144:VAL:HG23	1:C:245:PHE:HE1	1.84	0.41
1:D:26:THR:O	1:D:29:LYS:HG3	2.20	0.41
1:C:142:SER:HB3	1:C:381:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ASP:O	1:D:234:LYS:HB2	2.20	0.41
1:D:113:ASN:OD1	1:D:115:GLN:HB3	2.20	0.41
1:A:101:ASN:OD1	1:A:130:MET:HA	2.21	0.41
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.55	0.41
1:A:362:VAL:HA	1:A:365:LEU:HD22	2.01	0.41
1:B:391:ILE:CG2	1:C:279:LEU:HD21	2.50	0.41
1:C:307:LEU:HD12	1:C:310:MET:HE3	2.01	0.41
1:B:50:VAL:O	1:B:54:ARG:HG3	2.20	0.41
1:A:13:SER:O	1:D:12:PHE:HA	2.21	0.41
1:B:217:GLN:HB2	3:B:2059:HOH:O	2.20	0.41
1:D:266:LEU:C	1:D:266:LEU:HD23	2.45	0.41
1:D:362:VAL:HA	1:D:365:LEU:HD12	2.02	0.41
1:D:378:THR:O	1:D:382:GLN:HG2	2.20	0.41
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.56	0.41
1:A:23:PHE:CE2	1:A:75:LEU:HD21	2.57	0.40
1:D:312:TYR:CD1	1:D:312:TYR:C	3.00	0.40
1:D:377:GLY:HA3	1:D:382:GLN:HE21	1.85	0.40
1:B:368:ASP:O	1:B:371:ILE:HD11	2.21	0.40
1:B:120:TYR:CD1	1:B:198:ILE:HD11	2.57	0.40
1:C:366:MET:HB3	1:D:215:MET:CE	2.51	0.40
1:D:101:ASN:HA	1:D:131:CYS:SG	2.62	0.40
1:D:377:GLY:HA3	1:D:382:GLN:NE2	2.37	0.40
1:B:256:ARG:NE	1:B:382:GLN:HE22	2.19	0.40
1:C:106:MET:HE3	1:C:254:LYS:HB3	2.03	0.40
1:A:144:VAL:O	1:A:147:ILE:HG23	2.21	0.40
1:B:183:ASP:HA	1:B:184:PRO:HD2	1.92	0.40
1:B:187:LYS:HE3	1:B:187:LYS:HB3	1.92	0.40
1:C:136:THR:CG2	1:C:137:GLU:N	2.83	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%)	357 (93%)	26 (7%)	2 (0%)	24	37
1	B	385/396 (97%)	370 (96%)	15 (4%)	0	100	100
1	C	385/396 (97%)	370 (96%)	13 (3%)	2 (0%)	24	37
1	D	385/396 (97%)	355 (92%)	28 (7%)	2 (0%)	24	37
All	All	1540/1584 (97%)	1452 (94%)	82 (5%)	6 (0%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	D	166	TRP
1	D	193	ALA
1	A	141	GLY
1	C	141	GLY
1	C	192	LYS

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	303/310 (98%)	275 (91%)	28 (9%)	8	14
1	B	303/310 (98%)	280 (92%)	23 (8%)	12	21
1	C	303/310 (98%)	276 (91%)	27 (9%)	9	15
1	D	303/310 (98%)	268 (88%)	35 (12%)	5	8
All	All	1212/1240 (98%)	1099 (91%)	113 (9%)	8	14

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	62	MET
1	A	99	GLU
1	A	103	LEU
1	A	124	MET

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Mol	Chain	Res	Type
1	A	127	GLU
1	A	129	LEU
1	A	137	GLU
1	A	156	ASP
1	A	159	ILE
1	A	178	LEU
1	A	192	LYS
1	A	230	VAL
1	A	236	ASN
1	A	239	ILE
1	A	249	MET
1	A	255	GLU
1	A	258	VAL
1	A	268	GLN
1	A	298	LEU
1	A	312	TYR
1	A	319	VAL
1	A	324	ARG
1	A	333	LYS
1	A	359	GLU
1	A	365	LEU
1	A	375	TYR
1	A	381	ILE
1	B	10	LEU
1	B	75	LEU
1	B	115	GLN
1	B	121	LEU
1	B	161	ASN
1	B	163	GLN
1	B	179	LEU
1	B	198	ILE
1	B	199	VAL
1	B	217	GLN
1	B	258	VAL
1	B	271	LEU
1	B	279	LEU
1	B	281	ARG
1	B	288	LEU
1	B	307	LEU
1	B	319	VAL
1	B	348	VAL
1	B	351	LEU

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Mol	Chain	Res	Type
1	B	371	ILE
1	B	375	TYR
1	B	378	THR
1	B	381	ILE
1	C	69	ASN
1	C	92	THR
1	C	103	LEU
1	C	118	LYS
1	C	142	SER
1	C	152	GLU
1	C	154	LYS
1	C	161	ASN
1	C	179	LEU
1	C	192	LYS
1	C	210	ARG
1	C	238	LEU
1	C	254	LYS
1	C	255	GLU
1	C	286	LYS
1	C	287	LEU
1	C	290	GLU
1	C	295	SER
1	C	298	LEU
1	C	307	LEU
1	C	325	ASN
1	C	348	VAL
1	C	358	THR
1	C	365	LEU
1	C	371	ILE
1	C	375	TYR
1	C	396	ASN
1	D	19	GLN
1	D	47	GLU
1	D	48	TYR
1	D	55	ARG
1	D	58	GLU
1	D	73	LEU
1	D	75	LEU
1	D	85	GLU
1	D	92	THR
1	D	156	ASP
1	D	165	MET

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Mol	Chain	Res	Type
1	D	191	ASN
1	D	198	ILE
1	D	199	VAL
1	D	207	GLN
1	D	238	LEU
1	D	246	LYS
1	D	253	ASP
1	D	256	ARG
1	D	282	LYS
1	D	288	LEU
1	D	295	SER
1	D	314	ARG
1	D	319	VAL
1	D	324	ARG
1	D	325	ASN
1	D	326	THR
1	D	343	LEU
1	D	350	ILE
1	D	371	ILE
1	D	375	TYR
1	D	381	ILE
1	D	383	ARG
1	D	392	ASP
1	D	396	ASN

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

Mol	Chain	Res	Type
1	A	20	GLN
1	A	63	ASN
1	A	174	ASN
1	A	207	GLN
1	A	217	GLN
1	A	236	ASN
1	A	268	GLN
1	A	341	ASN
1	A	342	GLN
1	B	105	GLN
1	B	161	ASN
1	B	163	GLN
1	B	268	GLN
1	B	341	ASN

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Mol	Chain	Res	Type
1	B	373	GLN
1	B	382	GLN
1	C	63	ASN
1	C	65	HIS
1	C	69	ASN
1	C	95	GLN
1	C	116	GLN
1	C	161	ASN
1	C	169	ASN
1	C	207	GLN
1	C	268	GLN
1	C	313	GLN
1	C	325	ASN
1	C	341	ASN
1	C	354	ASN
1	C	382	GLN
1	D	20	GLN
1	D	95	GLN
1	D	105	GLN
1	D	115	GLN
1	D	169	ASN
1	D	174	ASN
1	D	207	GLN
1	D	236	ASN
1	D	268	GLN
1	D	349	GLN
1	D	354	ASN
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	B	399	-	58,58,58	1.25	6 (10%)	85,89,89	1.40	11 (12%)
2	FAD	A	399	-	58,58,58	1.11	2 (3%)	85,89,89	1.28	9 (10%)
2	FAD	C	399	-	58,58,58	1.19	4 (6%)	85,89,89	1.26	9 (10%)
2	FAD	D	399	-	58,58,58	1.24	5 (8%)	85,89,89	1.16	6 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	399	-	-	3/34/50/50	0/6/6/6
2	FAD	A	399	-	-	0/34/50/50	0/6/6/6
2	FAD	C	399	-	-	5/34/50/50	0/6/6/6
2	FAD	D	399	-	-	0/34/50/50	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	399	FAD	C9-C8	-3.99	1.34	1.39
2	B	399	FAD	C9-C8	-3.98	1.34	1.39
2	C	399	FAD	C10-N10	3.86	1.45	1.37
2	A	399	FAD	C4X-N5	3.68	1.38	1.30
2	D	399	FAD	C9-C8	-3.53	1.34	1.39
2	D	399	FAD	C4X-N5	3.44	1.38	1.30
2	D	399	FAD	C10-N10	3.42	1.44	1.37
2	B	399	FAD	C10-N10	3.21	1.44	1.37
2	C	399	FAD	C4X-N5	3.20	1.37	1.30
2	B	399	FAD	C6-C7	-3.02	1.35	1.39
2	C	399	FAD	C9-C8	-2.97	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	FAD	C4X-N5	2.65	1.36	1.30
2	B	399	FAD	C10-N1	2.33	1.37	1.33
2	C	399	FAD	C6-C7	-2.26	1.36	1.39
2	B	399	FAD	C5A-C4A	-2.17	1.35	1.39
2	D	399	FAD	C7M-C7	2.10	1.54	1.51
2	D	399	FAD	P-O2P	-2.09	1.45	1.55

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	399	FAD	C9A-C5X-N5	5.06	127.83	122.45
2	D	399	FAD	C9A-C5X-N5	4.42	127.14	122.45
2	B	399	FAD	C9A-C5X-N5	4.41	127.13	122.45
2	A	399	FAD	C9A-C5X-N5	3.72	126.40	122.45
2	A	399	FAD	C5X-N5-C4X	-3.57	112.31	118.09
2	B	399	FAD	O4'-C4'-C3'	-3.55	100.95	109.25
2	B	399	FAD	O3'-C3'-C4'	-3.49	101.01	108.93
2	B	399	FAD	C4'-C3'-C2'	3.33	119.11	113.57
2	B	399	FAD	C5X-N5-C4X	-3.26	112.81	118.09
2	A	399	FAD	C2B-C1B-N9A	-3.25	105.22	113.30
2	D	399	FAD	O5'-C5'-C4'	3.25	118.03	109.36
2	C	399	FAD	C5X-N5-C4X	-3.17	112.96	118.09
2	A	399	FAD	O5B-C5B-C4B	3.05	119.39	108.99
2	B	399	FAD	C2B-C3B-C4B	-2.92	96.97	102.61
2	D	399	FAD	C5X-N5-C4X	-2.82	113.52	118.09
2	C	399	FAD	O5B-C5B-C4B	2.78	118.46	108.99
2	A	399	FAD	O4'-C4'-C3'	2.64	115.43	109.25
2	D	399	FAD	O4-C4-N3	-2.63	115.18	120.11
2	D	399	FAD	O3B-C3B-C2B	-2.62	103.43	111.82
2	A	399	FAD	O4-C4-N3	-2.58	115.26	120.11
2	C	399	FAD	O4-C4-N3	-2.55	115.32	120.11
2	B	399	FAD	O2-C2-N1	2.52	125.98	121.80
2	B	399	FAD	C4-C4X-N5	-2.36	114.95	118.21
2	A	399	FAD	O4B-C1B-N9A	2.33	112.57	108.09
2	B	399	FAD	O4B-C1B-N9A	2.29	112.48	108.09
2	B	399	FAD	O4B-C1B-C2B	-2.26	101.78	106.62
2	C	399	FAD	C6-C5X-N5	-2.25	114.72	118.44
2	C	399	FAD	O2P-P-O3P	2.24	113.32	107.27
2	D	399	FAD	O2A-PA-O1A	2.22	122.78	112.44
2	C	399	FAD	C4A-N9A-C8A	-2.22	103.41	105.74
2	C	399	FAD	C1'-N10-C9A	-2.19	116.37	120.63
2	A	399	FAD	O2A-PA-O1A	2.13	122.37	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	399	FAD	C2B-C3B-C4B	-2.08	98.58	102.61
2	B	399	FAD	O4-C4-N3	-2.05	116.26	120.11
2	C	399	FAD	C4-C4X-N5	-2.00	115.44	118.21

There are no chirality outliers.

All (8) torsion outliers are listed below:

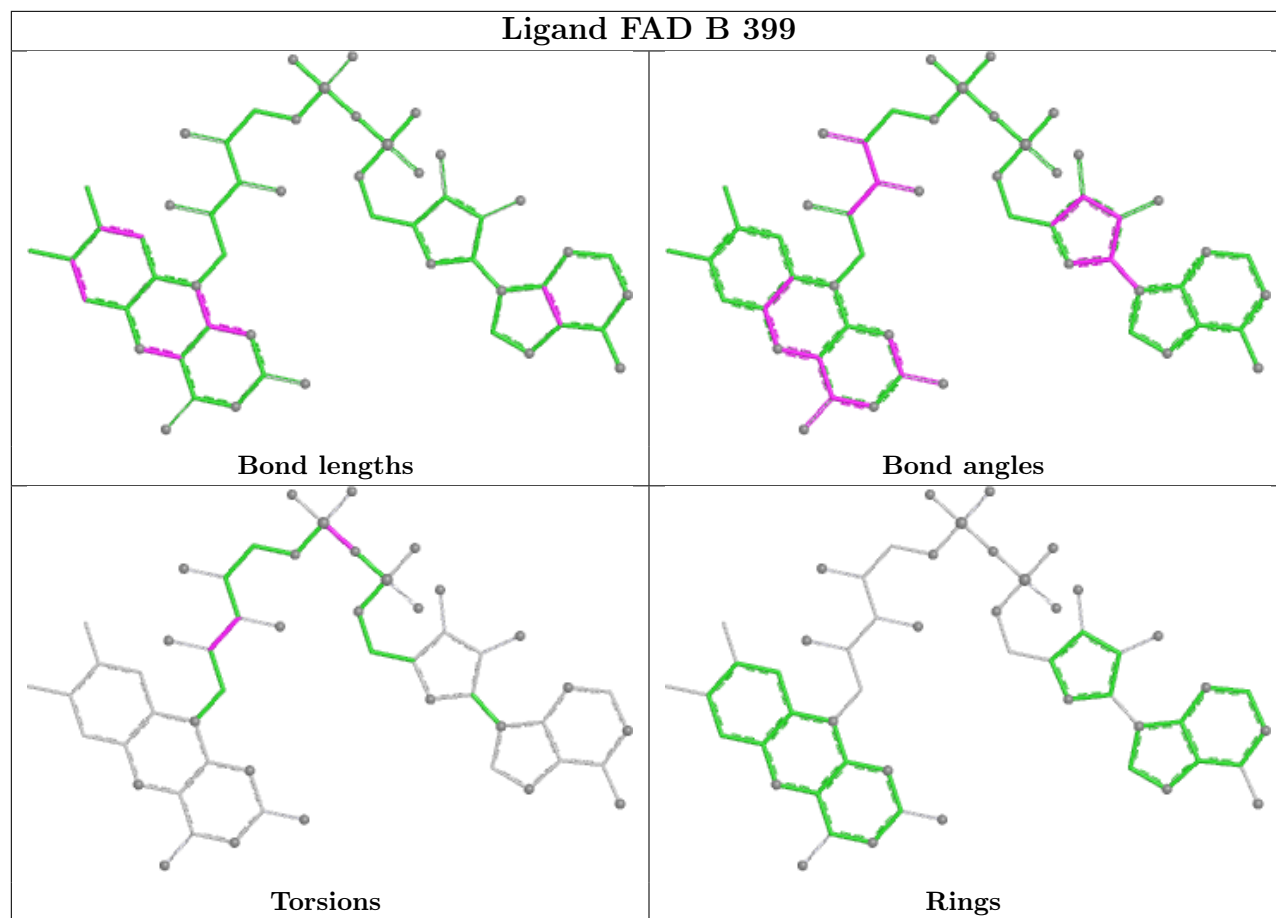
Mol	Chain	Res	Type	Atoms
2	C	399	FAD	C5'-O5'-P-O2P
2	C	399	FAD	C5'-O5'-P-O3P
2	C	399	FAD	C5'-O5'-P-O1P
2	B	399	FAD	PA-O3P-P-O2P
2	C	399	FAD	PA-O3P-P-O2P
2	B	399	FAD	O2'-C2'-C3'-O3'
2	B	399	FAD	PA-O3P-P-O1P
2	C	399	FAD	PA-O3P-P-O1P

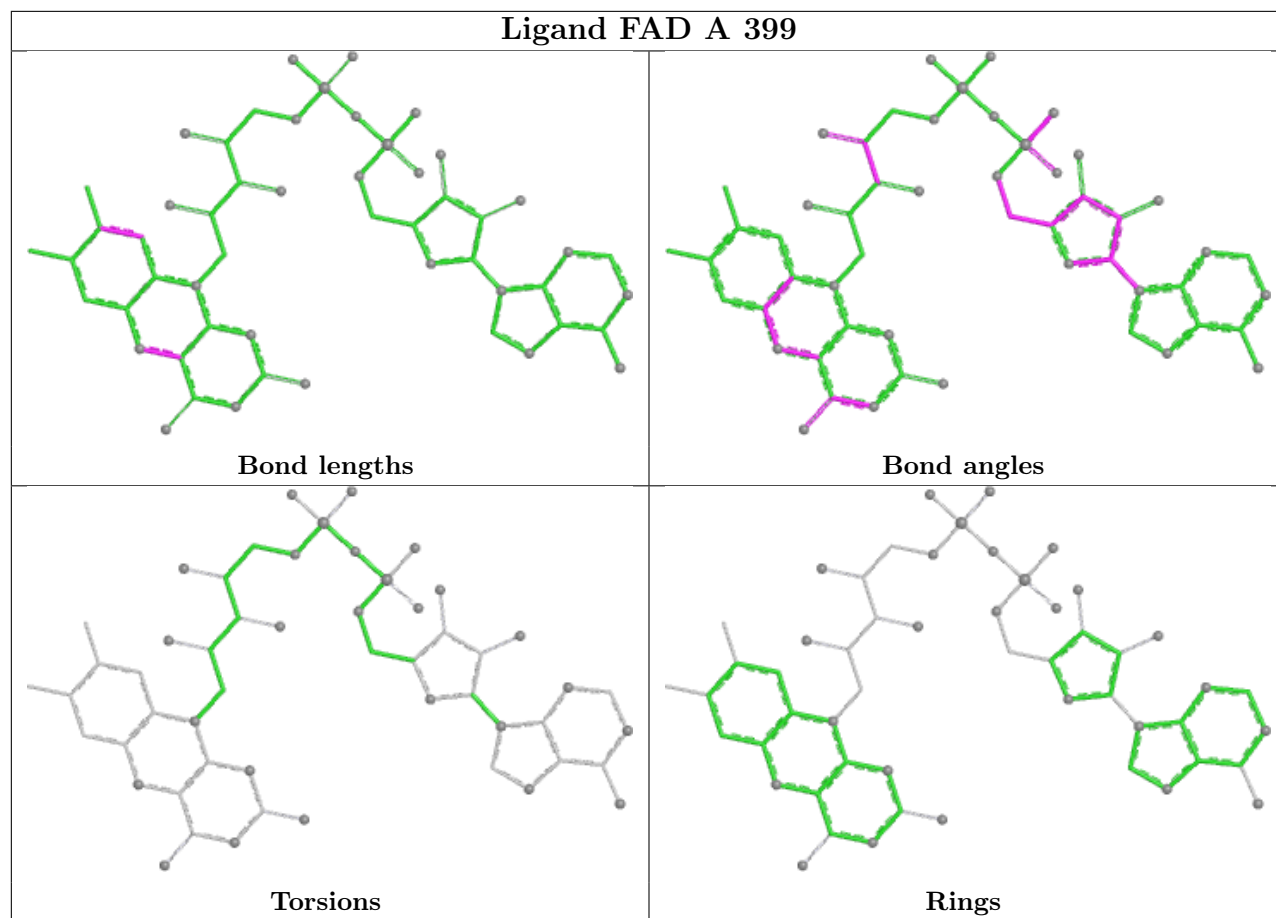
There are no ring outliers.

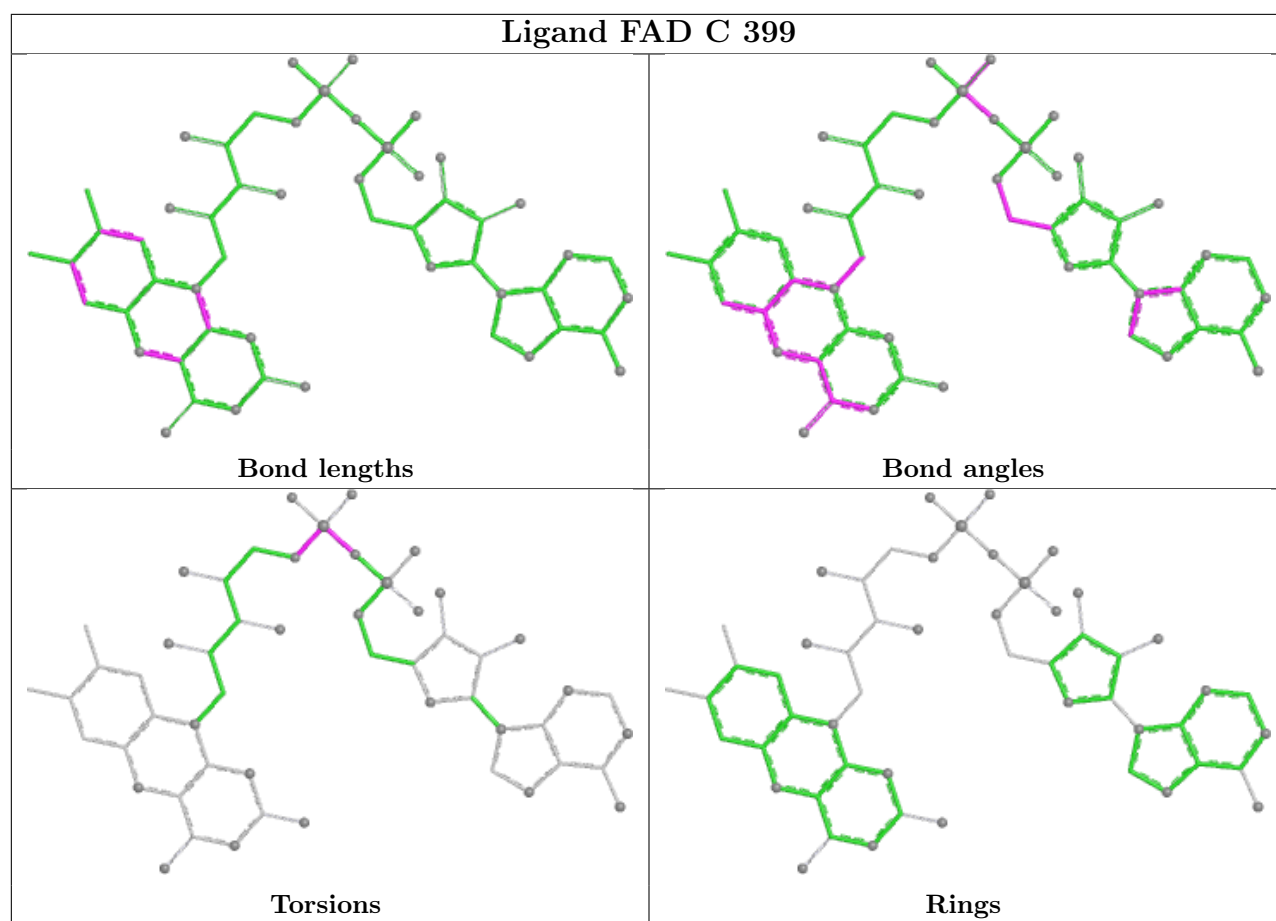
4 monomers are involved in 4 short contacts:

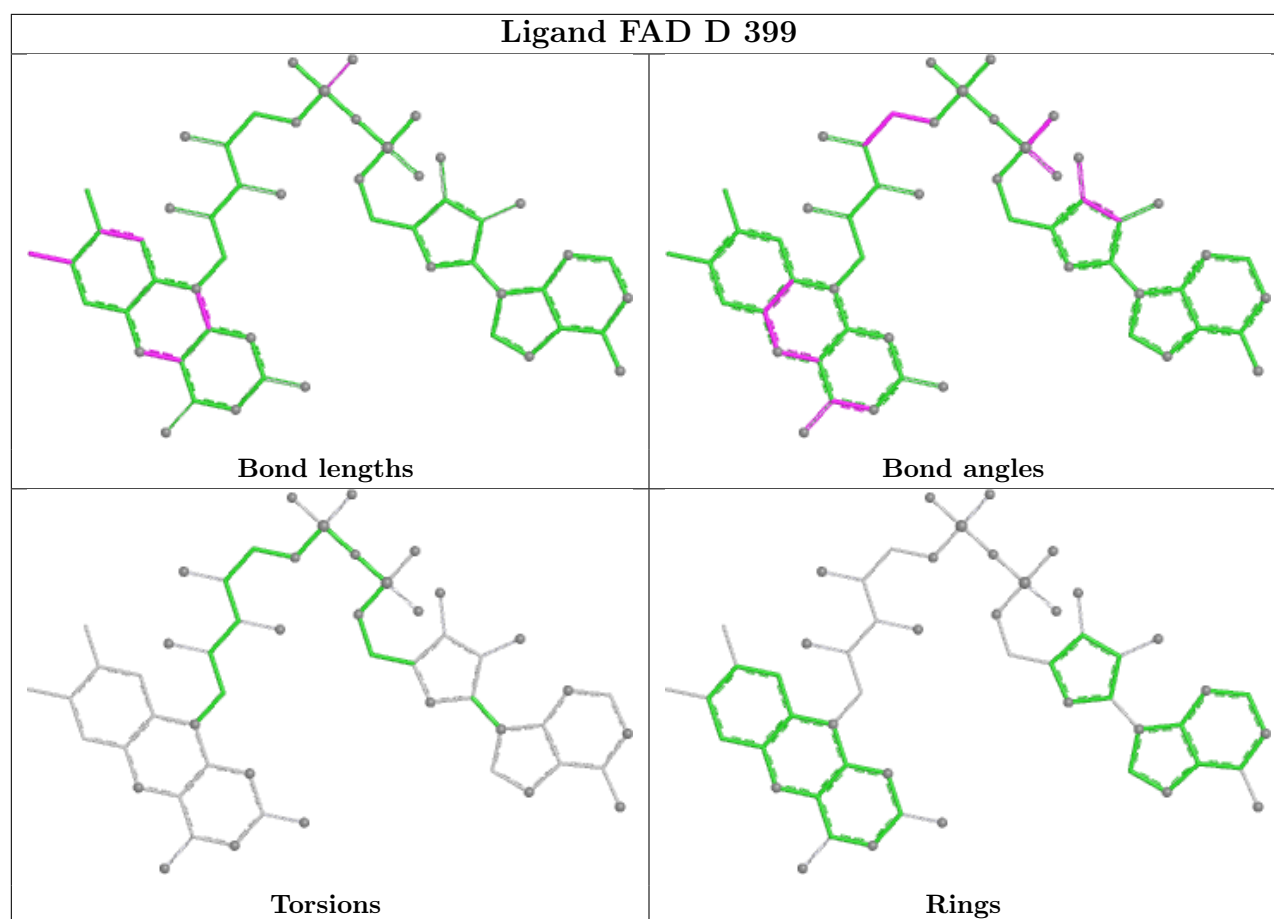
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	399	FAD	1	0
2	A	399	FAD	1	0
2	C	399	FAD	1	0
2	D	399	FAD	1	0

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.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	260:ALA	C	261:ALA	N	1.72
1	A	226:VAL	C	227:PHE	N	1.19
1	D	281:ARG	C	282:LYS	N	1.19
1	A	282:LYS	C	283:THR	N	1.15
1	A	240:GLY	C	241:ASP	N	1.03

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.