Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2024 – 02:35 PM EST

PDB ID	:	1EGE
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:

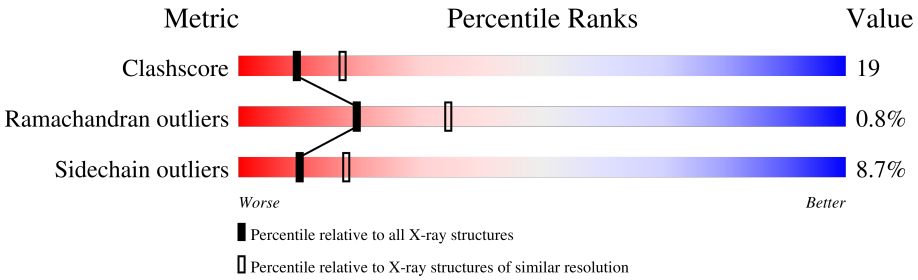
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	53% 39% 5% • •
1	B	396	62% 31% • • •
1	C	396	56% 37% 5% •
1	D	396	49% 41% 8% •

2 Entry composition (i)

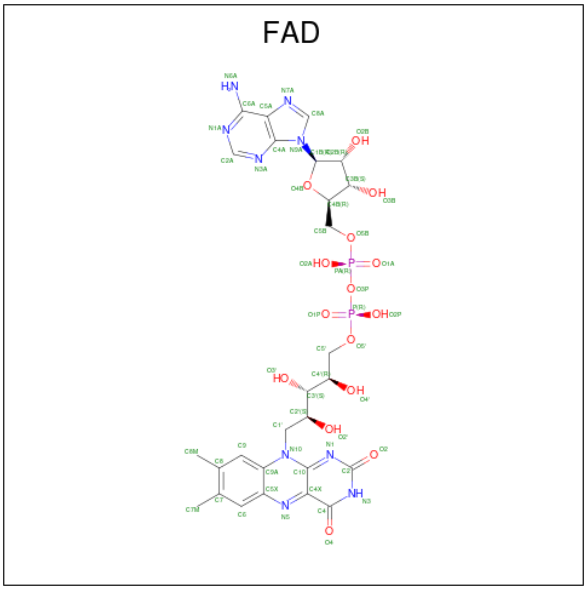
There are 2 unique types of molecules in this entry. The entry contains 12184 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (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		

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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		

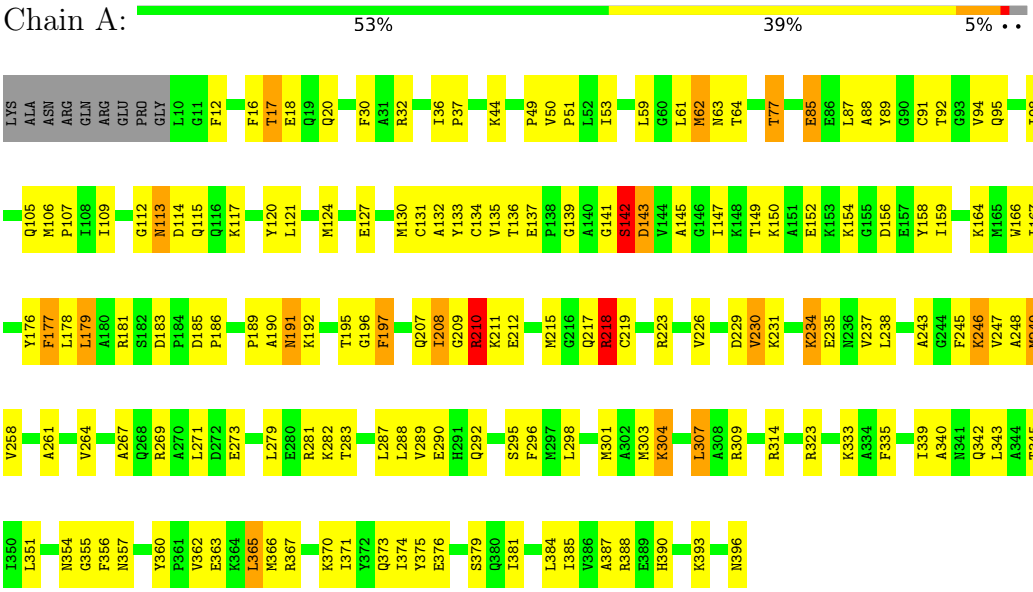
3 Residue-property plots (i)

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.

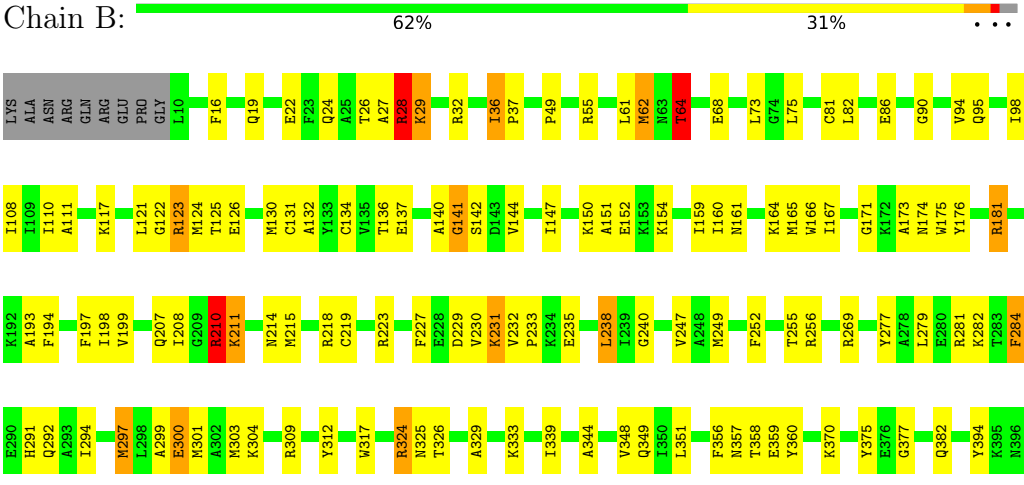
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain A:



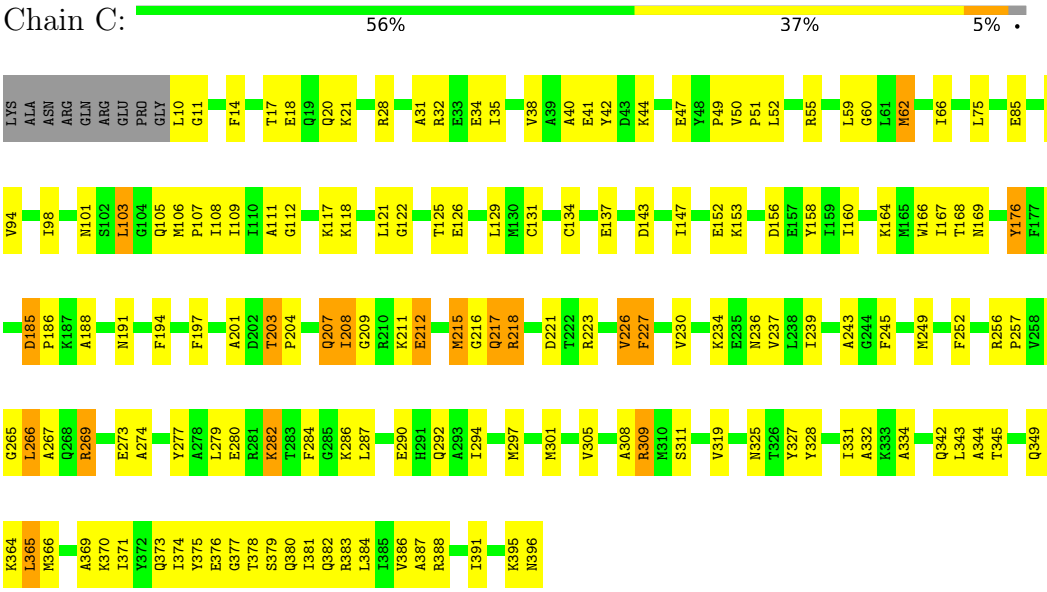
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain B:



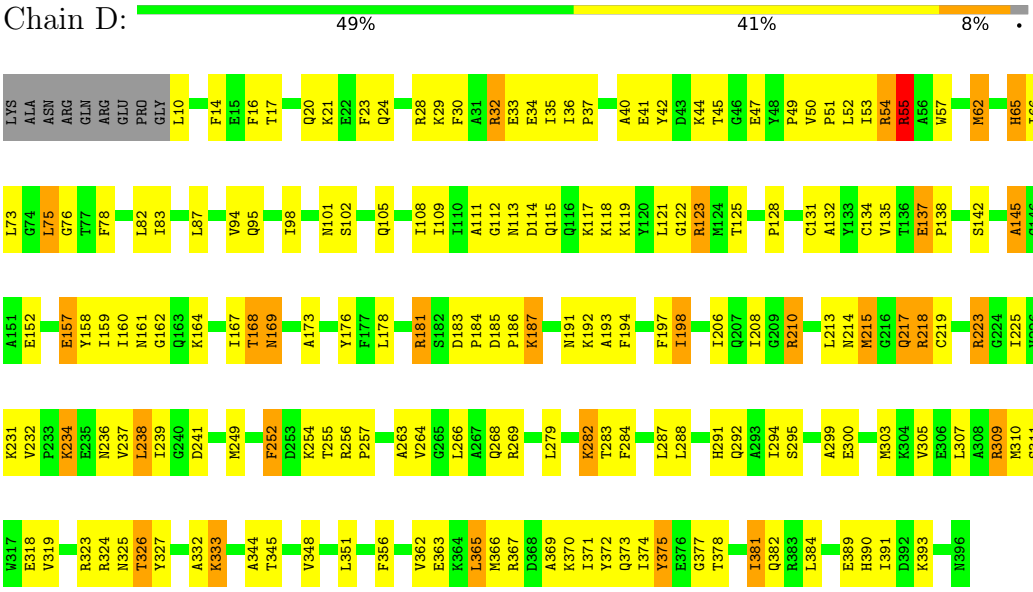
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain C:



• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D:



4 Data and refinement statistics (i)

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	0.49	0/3048	0.86	15/4107 (0.4%)
1	B	1.42	2/3048 (0.1%)	1.79	18/4107 (0.4%)
1	C	0.74	4/3048 (0.1%)	1.01	10/4107 (0.2%)
1	D	0.68	4/3048 (0.1%)	0.84	11/4107 (0.3%)
All	All	0.90	10/12192 (0.1%)	1.19	54/16428 (0.3%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	284	PHE	CD2-CE2	69.95	2.79	1.39
1	C	284	PHE	CG-CD1	23.19	1.73	1.38
1	C	284	PHE	CG-CD2	-16.62	1.13	1.38
1	B	324	ARG	C-N	-14.74	1.00	1.34
1	D	214	ASN	C-N	-8.39	1.14	1.34
1	C	60	GLY	C-N	7.51	1.51	1.34
1	C	226	VAL	C-N	-6.60	1.18	1.34
1	D	169	ASN	CG-ND2	-6.54	1.16	1.32
1	D	32	ARG	C-N	5.93	1.47	1.34
1	D	76	GLY	N-CA	5.70	1.54	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	284	PHE	CE1-CZ-CE2	-65.95	1.28	120.00
1	B	284	PHE	CG-CD2-CE2	-55.57	59.67	120.80
1	B	284	PHE	CZ-CE2-CD2	-49.75	60.40	120.10
1	C	284	PHE	CB-CG-CD2	31.16	142.61	120.80
1	C	284	PHE	CB-CG-CD1	-24.65	103.54	120.80
1	A	169	ASN	O-C-N	-15.36	97.08	123.20
1	A	169	ASN	CA-C-N	12.60	141.41	116.20
1	C	218	ARG	O-C-N	-12.18	103.22	122.70
1	B	324	ARG	C-N-CA	12.14	152.06	121.70
1	D	218	ARG	O-C-N	-9.81	107.01	122.70
1	C	284	PHE	CG-CD2-CE2	9.13	130.84	120.80
1	A	64	THR	O-C-N	-9.09	108.16	122.70
1	B	64	THR	O-C-N	-8.70	108.78	122.70
1	A	218	ARG	O-C-N	-7.91	110.05	122.70
1	B	324	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	D	218	ARG	NE-CZ-NH2	7.34	123.97	120.30
1	B	218	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	A	218	ARG	NE-CZ-NH2	7.22	123.91	120.30
1	B	28	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	C	218	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	D	168	THR	O-C-N	7.09	134.05	122.70
1	A	210	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	D	218	ARG	CA-C-N	6.99	132.59	117.20
1	B	210	ARG	NE-CZ-NH2	6.73	123.67	120.30
1	B	123	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	D	47	GLU	O-C-N	6.55	133.18	122.70
1	A	62	MET	CG-SD-CE	6.39	110.42	100.20
1	B	62	MET	CG-SD-CE	6.37	110.39	100.20
1	B	240	GLY	CA-C-N	-6.37	103.19	117.20
1	B	240	GLY	O-C-N	6.32	132.81	122.70
1	D	47	GLU	CA-C-N	-6.32	103.30	117.20
1	B	181	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	D	215	MET	CG-SD-CE	6.23	110.17	100.20
1	B	223	ARG	NE-CZ-NH2	6.21	123.40	120.30
1	A	215	MET	CG-SD-CE	6.17	110.08	100.20
1	C	218	ARG	CA-C-N	6.14	130.72	117.20
1	A	230	VAL	CA-C-N	-6.12	103.74	117.20
1	C	215	MET	CG-SD-CE	6.10	109.96	100.20
1	C	62	MET	CG-SD-CE	6.04	109.86	100.20
1	B	215	MET	CG-SD-CE	6.00	109.79	100.20
1	A	217	GLN	O-C-N	5.82	132.01	122.70
1	B	64	THR	CA-C-N	5.67	129.68	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	124	MET	CG-SD-CE	5.63	109.21	100.20
1	D	65	HIS	O-C-N	-5.52	113.87	122.70
1	A	64	THR	CA-C-N	5.47	129.23	117.20
1	D	62	MET	CG-SD-CE	5.39	108.82	100.20
1	C	236	ASN	O-C-N	-5.27	114.27	122.70
1	A	62	MET	O-C-N	5.27	131.13	122.70
1	D	112	GLY	O-C-N	5.26	131.12	122.70
1	A	217	GLN	CA-C-N	-5.22	105.72	117.20
1	C	60	GLY	C-N-CA	-5.15	108.82	121.70
1	A	218	ARG	CA-C-N	5.14	128.51	117.20
1	A	177	PHE	N-CA-C	-5.13	97.15	111.00
1	D	229	ASP	CA-C-N	-5.05	106.09	117.20

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2993	0	2982	123	0
1	B	2993	0	2981	116	0
1	C	2993	0	2981	118	0
1	D	2993	0	2981	146	0
2	A	53	0	31	6	0
2	B	53	0	31	1	0
2	C	53	0	31	5	0
2	D	53	0	31	1	0
All	All	12184	0	12049	472	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 19.

All (472) 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:NZ	1:A:304:LYS:HA	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: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
1:D:252:PHE:HA	1:D:255:THR:OG1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:304:LYS:HA	1:A:304:LYS:HZ2	1.54	0.69
1:B:199:VAL:HG22	1:B:232:VAL:HG11	1.73	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
1:D:197:PHE:CD2	1:D:237:VAL:HG22	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:34:GLU:OE1	1:D:34:GLU:HA	2.00	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: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:A:374:ILE:HG12	1:B:349:GLN:HE22	1.65	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: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:161:ASN:HD21	1:B:229:ASP:CG	2.07	0.58
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:376:GLU:HG3	1:C:376:GLU:O	2.06	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:166:TRP:CZ3	1:C:212:GLU:HG2	2.44	0.53
1:B:144:VAL:HG11	1:B:249:MET:HE3	1.91	0.52
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:249:MET:HE1	1:B:252:PHE:HE2	1.76	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:C:395:LYS:O	1:C:396:ASN:HB2	2.12	0.50
1:A:304:LYS:HA	1:A:304:LYS:HZ3	1.72	0.49
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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: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
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:A:245:PHE:O	1:A:249:MET:HB2	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:303:MET:O	1:D:307:LEU:HD13	2.16	0.46
1:C:208:ILE:CG2	1:C:209:GLY:N	2.75	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
1:A:371:ILE:HD13	2:A:399:FAD:HM83	1.97	0.45
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:351:LEU:HD22	1:D:362:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HB3	1:A:107:PRO:HD3	1.99	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: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:D:53:ILE:HG23	1:D:62:MET:HE1	1.99	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:D:326:THR:HG23	1:D:327:TYR:N	2.32	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:A:347:ALA:O	1:A:351:LEU:HD13	2.17	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:356:PHE:CD2	1:B:214:ASN:HB3	2.53	0.43
1:C:216:GLY:O	1:C:217:GLN:C	2.56	0.43
1:C:388:ARG:HD2	1:C:388:ARG:C	2.37	0.43
1:D:65:HIS:O	1:D:66:ILE:C	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:D:78:PHE:HA	1:D:316:ALA:HB1	2.02	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:A:185:ASP:HA	1:A:186:PRO:HD2	1.87	0.42
1:B:28:ARG:O	1:B:29:LYS:C	2.58	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:106:MET:HB2	1:C:106:MET:HE2	1.98	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: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:281:ARG:HG3	1:B:288:LEU:HD13	2.02	0.41
1:D:55:ARG:HG3	1:D:55:ARG:HH11	1.84	0.41
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:304:LYS:HZ2	1:A:335:PHE:HZ	1.68	0.41
1:A:373:GLN:HB3	1:B:349:GLN:OE1	2.21	0.41
1:B:358:THR:C	1:B:360:TYR:H	2.23	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: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:C:371:ILE:HD13	2:C:399:FAD:HM83	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:62:MET:HE3	1:B:130:MET:SD	2.61	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%)	15	27
1	B	385/396 (97%)	349 (91%)	34 (9%)	2 (0%)	29	47
1	C	385/396 (97%)	355 (92%)	29 (8%)	1 (0%)	41	60
1	D	385/396 (97%)	347 (90%)	33 (9%)	5 (1%)	12	21
All	All	1540/1584 (97%)	1394 (90%)	134 (9%)	12 (1%)	19	34

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 (i)

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%)	268 (88%)	36 (12%)	5 8
1	B	304/311 (98%)	283 (93%)	21 (7%)	15 27
1	C	304/311 (98%)	281 (92%)	23 (8%)	13 23
1	D	304/311 (98%)	278 (91%)	26 (9%)	10 18
All	All	1216/1244 (98%)	1110 (91%)	106 (9%)	10 18

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	THR
1	A	44	LYS
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
1	A	152	GLU
1	A	158	TYR
1	A	179	LEU
1	A	191	ASN
1	A	197	PHE
1	A	208	ILE
1	A	210	ARG
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	283	THR
1	A	295	SER
1	A	296	PHE
1	A	304	LYS
1	A	307	LEU
1	A	323	ARG
1	A	333	LYS
1	A	365	LEU
1	A	366	MET
1	A	375	TYR

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Mol	Chain	Res	Type
1	A	376	GLU
1	A	379	SER
1	A	396	ASN
1	B	28	ARG
1	B	36	ILE
1	B	55	ARG
1	B	64	THR
1	B	68	GLU
1	B	95	GLN
1	B	137	GLU
1	B	142	SER
1	B	185	ASP
1	B	197	PHE
1	B	207	GLN
1	B	210	ARG
1	B	211	LYS
1	B	231	LYS
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	375	TYR
1	C	41	GLU
1	C	75	LEU
1	C	103	LEU
1	C	118	LYS
1	C	126	GLU
1	C	129	LEU
1	C	152	GLU
1	C	176	TYR
1	C	179	LEU
1	C	181	ARG
1	C	185	ASP
1	C	203	THR
1	C	207	GLN
1	C	212	GLU
1	C	221	ASP
1	C	227	PHE
1	C	249	MET
1	C	266	LEU

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Mol	Chain	Res	Type
1	C	282	LYS
1	C	309	ARG
1	C	358	THR
1	C	365	LEU
1	C	375	TYR
1	D	24	GLN
1	D	54	ARG
1	D	55	ARG
1	D	75	LEU
1	D	94	VAL
1	D	95	GLN
1	D	102	SER
1	D	123	ARG
1	D	137	GLU
1	D	148	LYS
1	D	157	GLU
1	D	178	LEU
1	D	187	LYS
1	D	198	ILE
1	D	210	ARG
1	D	223	ARG
1	D	234	LYS
1	D	252	PHE
1	D	254	LYS
1	D	269	ARG
1	D	282	LYS
1	D	295	SER
1	D	333	LYS
1	D	365	LEU
1	D	375	TYR
1	D	381	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	105	GLN
1	A	116	GLN
1	A	191	ASN
1	A	341	ASN
1	A	342	GLN
1	A	349	GLN

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Mol	Chain	Res	Type
1	A	354	ASN
1	A	373	GLN
1	A	396	ASN
1	B	63	ASN
1	B	65	HIS
1	B	95	GLN
1	B	105	GLN
1	B	161	ASN
1	B	169	ASN
1	B	174	ASN
1	B	268	GLN
1	B	325	ASN
1	B	396	ASN
1	C	69	ASN
1	C	313	GLN
1	C	349	GLN
1	C	382	GLN
1	C	396	ASN
1	D	207	GLN
1	D	217	GLN
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 monosaccharides 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	D	399	-	53,58,58	1.49	7 (13%)	68,89,89	2.02	15 (22%)
2	FAD	C	399	-	53,58,58	1.22	3 (5%)	68,89,89	1.60	11 (16%)
2	FAD	A	399	-	53,58,58	1.36	7 (13%)	68,89,89	1.63	12 (17%)
2	FAD	B	399	-	53,58,58	1.30	6 (11%)	68,89,89	1.82	12 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	399	-	-	9/30/50/50	0/6/6/6
2	FAD	C	399	-	-	8/30/50/50	0/6/6/6
2	FAD	A	399	-	-	4/30/50/50	0/6/6/6
2	FAD	B	399	-	-	10/30/50/50	0/6/6/6

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	399	FAD	O4B-C1B	4.08	1.46	1.41
2	C	399	FAD	C9-C8	-3.96	1.33	1.39
2	D	399	FAD	C6-C7	-3.82	1.34	1.39
2	B	399	FAD	C4X-N5	3.80	1.38	1.30
2	A	399	FAD	C4X-N5	3.63	1.37	1.30
2	C	399	FAD	C4X-N5	3.51	1.37	1.30
2	D	399	FAD	C8A-N7A	-3.46	1.28	1.34
2	D	399	FAD	C5X-N5	-3.30	1.33	1.39
2	C	399	FAD	C10-N10	2.99	1.43	1.37
2	D	399	FAD	C9-C8	-2.95	1.35	1.39
2	D	399	FAD	C10-N10	2.92	1.43	1.37
2	A	399	FAD	C6-C7	-2.88	1.35	1.39
2	B	399	FAD	C8A-N7A	-2.87	1.29	1.34
2	A	399	FAD	C9-C8	-2.86	1.35	1.39
2	A	399	FAD	C10-N10	2.84	1.43	1.37
2	D	399	FAD	C4X-N5	2.84	1.36	1.30
2	B	399	FAD	O4B-C1B	2.75	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	FAD	C6-C7	-2.57	1.35	1.39
2	B	399	FAD	C9-C8	-2.51	1.35	1.39
2	A	399	FAD	C1'-N10	-2.47	1.41	1.48
2	B	399	FAD	C10-N10	2.41	1.42	1.37
2	A	399	FAD	C2-N3	-2.29	1.33	1.39
2	A	399	FAD	C10-N1	2.06	1.37	1.33

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	399	FAD	O4B-C1B-C2B	-5.99	98.17	106.93
2	B	399	FAD	O3'-C3'-C2'	-5.50	95.52	108.81
2	B	399	FAD	C9A-C5X-N5	5.28	128.17	122.43
2	C	399	FAD	C2B-C3B-C4B	-5.05	92.82	102.64
2	D	399	FAD	C9A-C5X-N5	4.76	127.61	122.43
2	C	399	FAD	O4B-C1B-C2B	-4.56	100.26	106.93
2	B	399	FAD	O4B-C1B-C2B	-4.32	100.62	106.93
2	D	399	FAD	O3'-C3'-C2'	4.21	118.98	108.81
2	D	399	FAD	C2B-C3B-C4B	-4.21	94.47	102.64
2	B	399	FAD	C5X-N5-C4X	-4.02	111.39	118.07
2	B	399	FAD	P-O3P-PA	-4.01	119.06	132.83
2	D	399	FAD	C3B-C2B-C1B	3.99	106.98	100.98
2	A	399	FAD	O4-C4-N3	-3.86	112.71	120.12
2	A	399	FAD	O3'-C3'-C2'	-3.86	99.49	108.81
2	D	399	FAD	C6-C5X-N5	-3.86	111.78	118.51
2	B	399	FAD	O5B-C5B-C4B	3.81	122.10	108.99
2	A	399	FAD	C9A-C5X-N5	3.80	126.56	122.43
2	B	399	FAD	C4-C4X-N5	-3.75	112.89	118.23
2	D	399	FAD	C4-C4X-N5	-3.67	113.01	118.23
2	A	399	FAD	O2-C2-N1	3.56	127.73	121.83
2	C	399	FAD	O2-C2-N1	3.55	127.71	121.83
2	D	399	FAD	O4B-C4B-C3B	3.46	111.96	105.11
2	A	399	FAD	O4B-C4B-C3B	-3.37	98.44	105.11
2	D	399	FAD	C1B-N9A-C4A	3.34	132.51	126.64
2	A	399	FAD	O4B-C1B-C2B	-3.33	102.06	106.93
2	C	399	FAD	C9A-C5X-N5	3.28	126.00	122.43
2	D	399	FAD	C5X-N5-C4X	-3.11	112.91	118.07
2	C	399	FAD	C5X-N5-C4X	-3.08	112.95	118.07
2	C	399	FAD	O4-C4-N3	-2.99	114.38	120.12
2	A	399	FAD	C2B-C3B-C4B	-2.87	97.07	102.64
2	A	399	FAD	C5X-N5-C4X	-2.86	113.31	118.07
2	D	399	FAD	O2'-C2'-C1'	-2.86	102.88	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	399	FAD	P-O3P-PA	-2.85	123.03	132.83
2	B	399	FAD	C3B-C2B-C1B	2.67	104.99	100.98
2	B	399	FAD	C4A-C5A-N7A	2.51	112.01	109.40
2	D	399	FAD	C7M-C7-C8	2.49	125.83	120.74
2	D	399	FAD	C4'-C3'-C2'	-2.43	108.30	113.36
2	A	399	FAD	O4'-C4'-C3'	2.37	114.87	109.10
2	B	399	FAD	C2B-C3B-C4B	-2.35	98.09	102.64
2	B	399	FAD	C6-C5X-N5	-2.29	114.52	118.51
2	C	399	FAD	C4-C4X-N5	-2.29	114.98	118.23
2	B	399	FAD	O4'-C4'-C5'	-2.27	104.82	109.92
2	C	399	FAD	O4'-C4'-C5'	-2.27	104.82	109.92
2	A	399	FAD	O2A-PA-O1A	2.25	123.39	112.24
2	C	399	FAD	C1'-N10-C9A	-2.23	116.80	120.51
2	C	399	FAD	PA-O5B-C5B	-2.21	108.72	121.68
2	D	399	FAD	O2A-PA-O1A	2.12	122.70	112.24
2	C	399	FAD	P-O5'-C5'	-2.11	109.31	121.68
2	A	399	FAD	C5A-C6A-N6A	2.09	123.53	120.35
2	A	399	FAD	C1'-N10-C9A	-2.07	117.06	120.51

There are no chirality outliers.

All (31) torsion outliers are listed below:

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

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

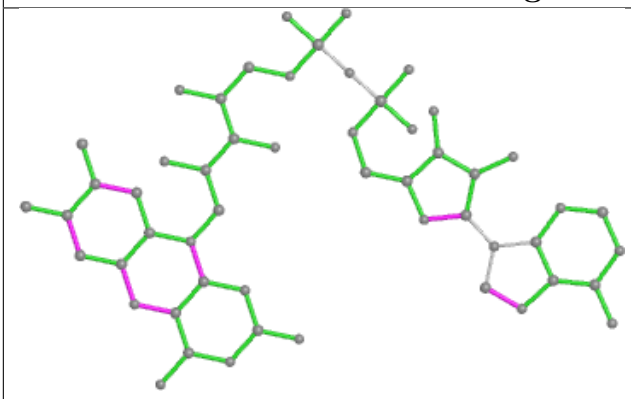
There are no ring outliers.

4 monomers are involved in 13 short contacts:

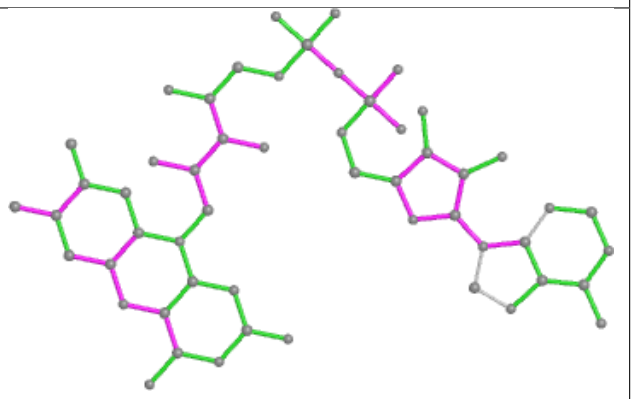
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	399	FAD	1	0
2	C	399	FAD	5	0
2	A	399	FAD	6	0
2	B	399	FAD	1	0

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 then 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.

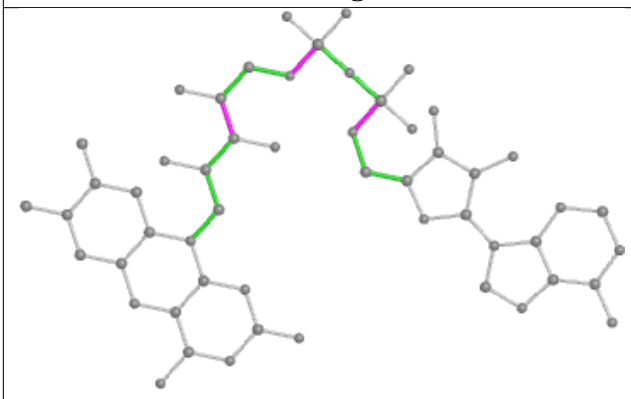
Ligand FAD D 399



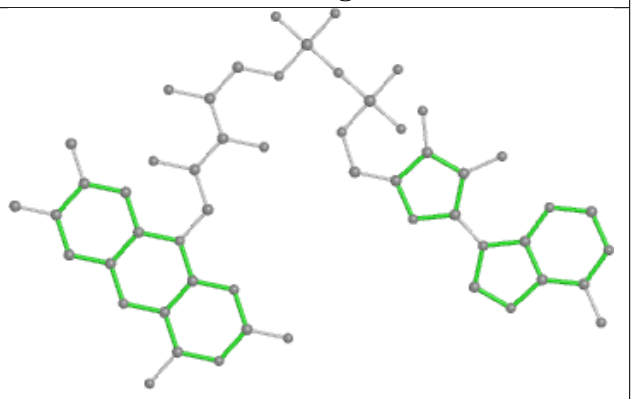
Bond lengths



Bond angles

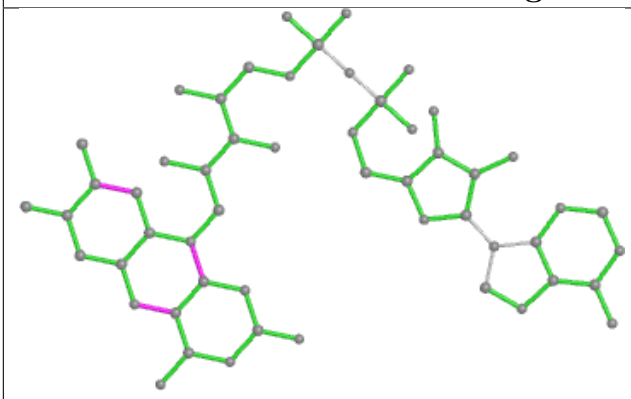


Torsions

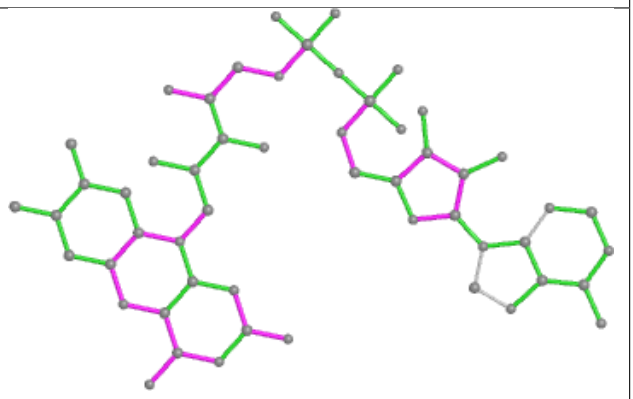


Rings

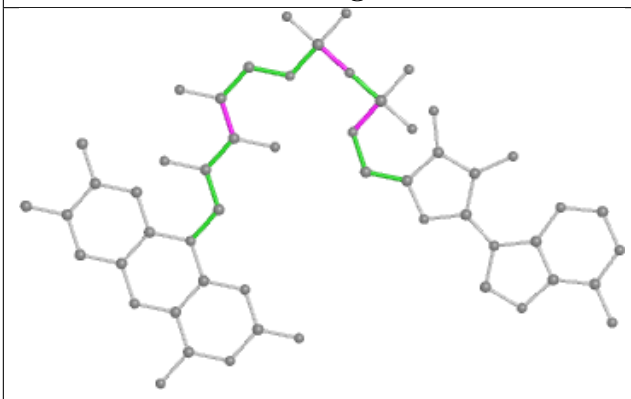
Ligand FAD C 399



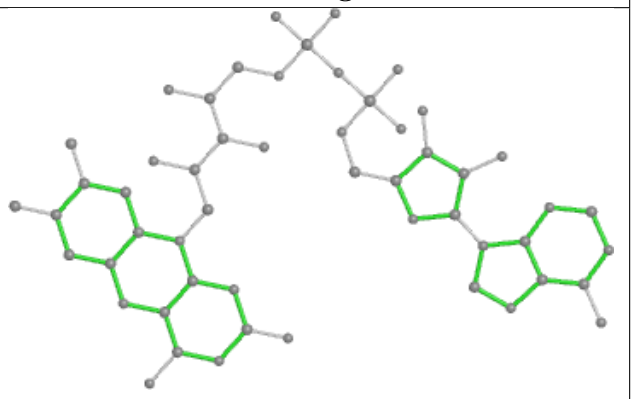
Bond lengths



Bond angles

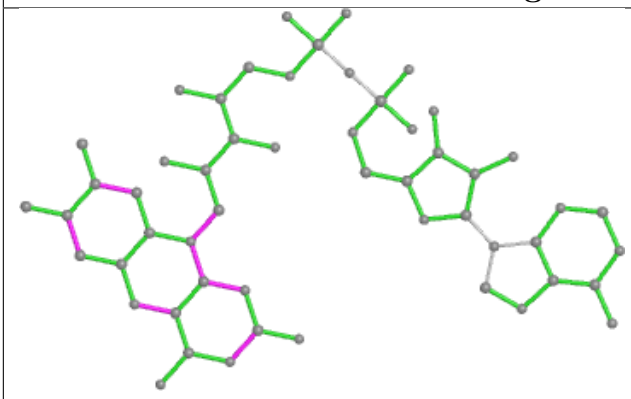


Torsions

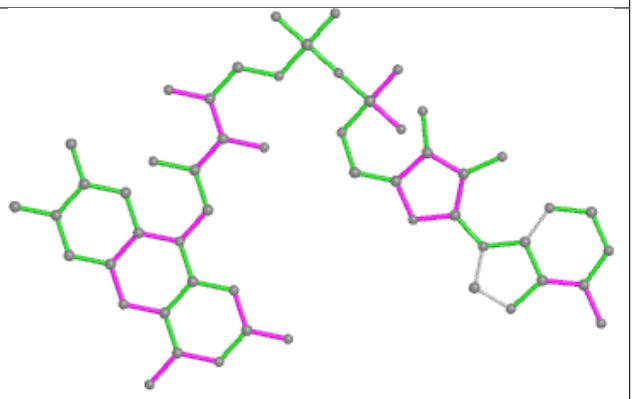


Rings

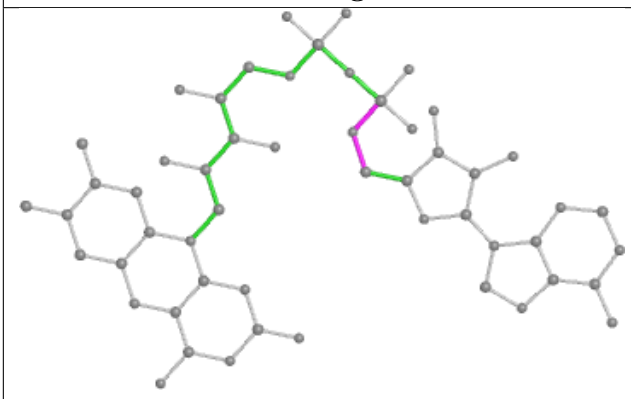
Ligand FAD A 399



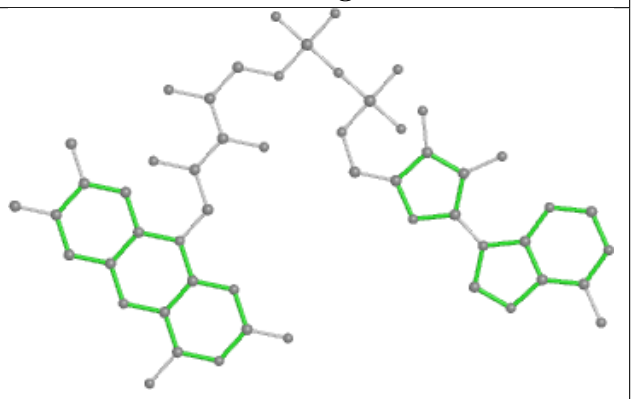
Bond lengths



Bond angles

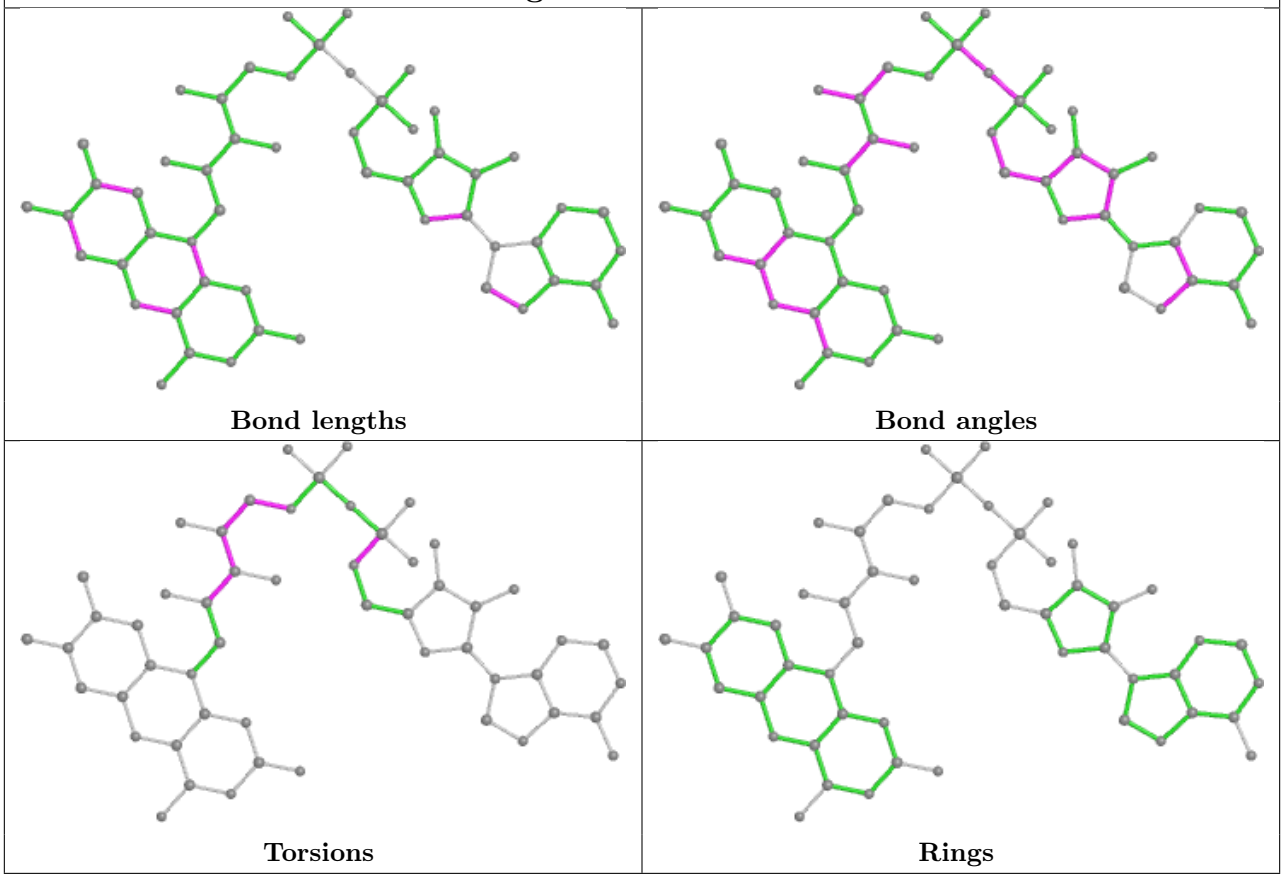


Torsions



Rings

Ligand FAD B 399



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	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.