



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:11 PM GMT

PDB ID : 1EGD
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

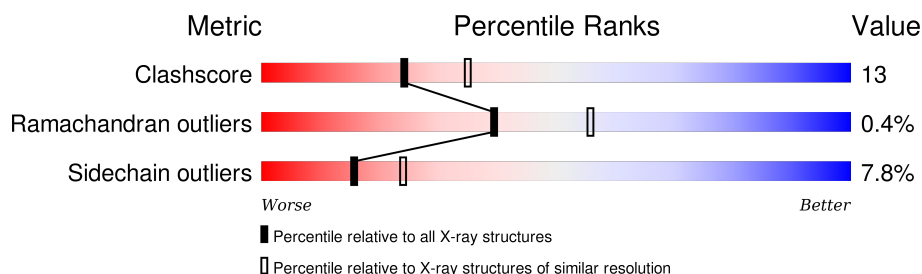
1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	396	 66% 27% . . .
1	B	396	 71% 23% . .
1	C	396	 69% 25% . .
1	D	396	 58% 33% 7% . .

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	UNP P11310
A	376	GLY	GLU	ENGINEERED	UNP P11310
B	255	GLU	THR	ENGINEERED	UNP P11310
B	376	GLY	GLU	ENGINEERED	UNP P11310
C	255	GLU	THR	ENGINEERED	UNP P11310
C	376	GLY	GLU	ENGINEERED	UNP P11310
D	255	GLU	THR	ENGINEERED	UNP P11310
D	376	GLY	GLU	ENGINEERED	UNP P11310

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



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

- Molecule 3 is water.

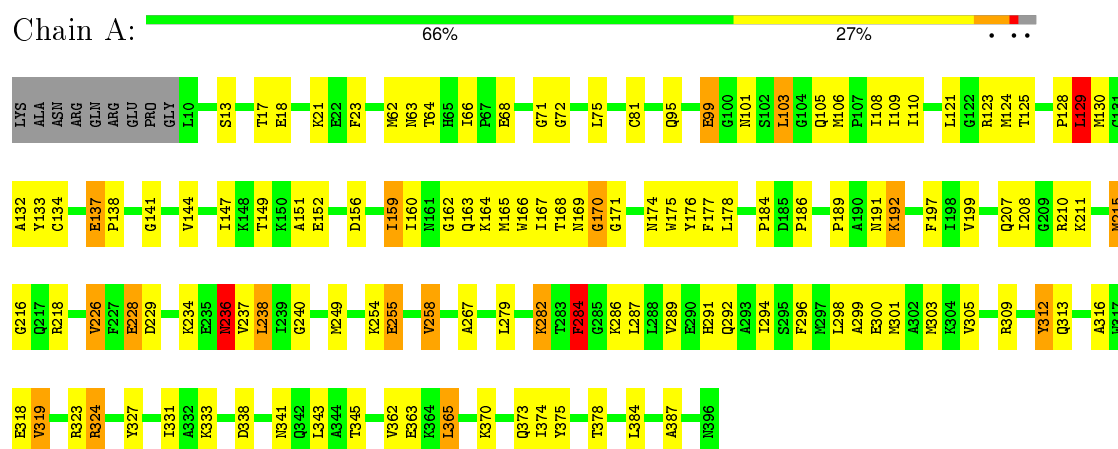
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	61	Total	O	0	0
			61	61		
3	C	68	Total	O	0	0
			68	68		
3	D	44	Total	O	0	0
			44	44		

3 Residue-property plots

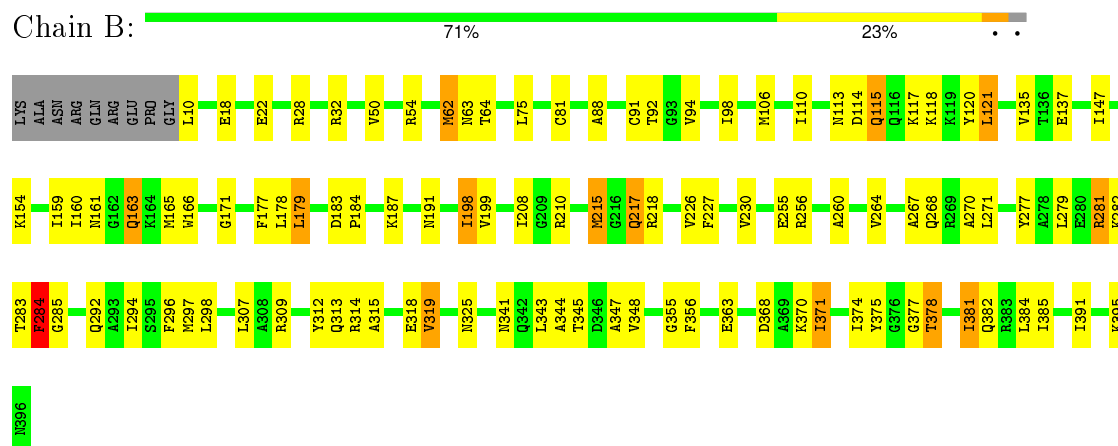
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

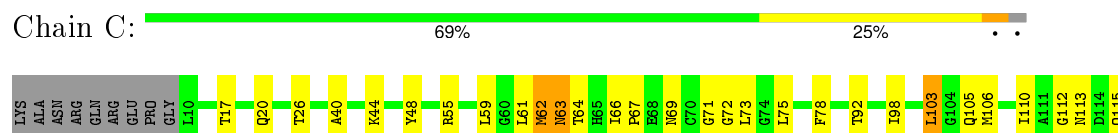
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

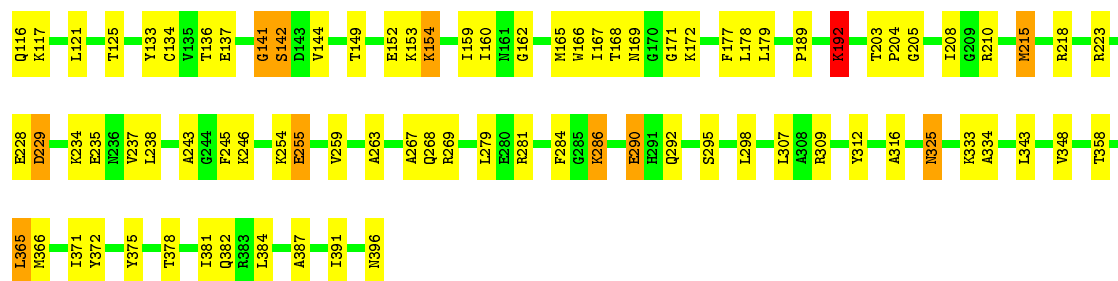


• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE



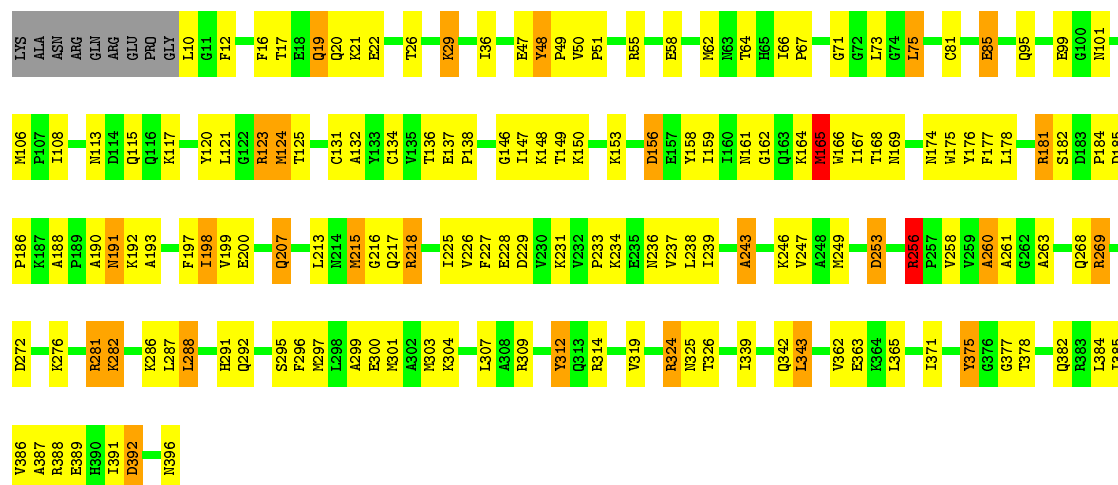
• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE





• Molecule 1: MEDIUM CHAIN ACYL-COA DEHYDROGENASE

Chain D: 58% 33% 7% ..



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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 ⓘ

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	1.42	7/3045 (0.2%)	1.75	18/4102 (0.4%)
1	B	0.50	2/3045 (0.1%)	0.81	13/4102 (0.3%)
1	C	0.48	2/3045 (0.1%)	0.78	11/4102 (0.3%)
1	D	0.65	3/3045 (0.1%)	0.84	13/4102 (0.3%)
All	All	0.85	14/12180 (0.1%)	1.12	55/16408 (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	4
All	All	0	12

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PHE	CD1-CE1	70.04	2.79	1.39
1	D	260	ALA	C-N	16.50	1.72	1.34
1	A	240	GLY	C-N	-13.25	1.03	1.34
1	A	282	LYS	C-N	-8.22	1.15	1.34
1	B	395	LYS	C-N	7.15	1.50	1.34
1	A	226	VAL	C-N	-6.52	1.19	1.34
1	D	281	ARG	C-N	-6.25	1.19	1.34
1	A	236	ASN	C-N	5.88	1.47	1.34
1	C	281	ARG	C-N	-5.75	1.20	1.34
1	A	128	PRO	C-N	-5.58	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	129	LEU	N-CA	-5.55	1.35	1.46
1	D	243	ALA	C-N	-5.30	1.23	1.33
1	B	284	PHE	C-N	5.11	1.42	1.33
1	C	205	GLY	N-CA	5.09	1.53	1.46

All (55) 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	-55.06	60.24	120.80
1	A	284	PHE	CD1-CE1-CZ	-49.73	60.42	120.10
1	B	395	LYS	O-C-N	13.52	144.33	122.70
1	C	64	THR	O-C-N	-11.64	104.08	122.70
1	A	218	ARG	O-C-N	-10.57	105.79	122.70
1	B	395	LYS	CA-C-N	-9.88	95.48	117.20
1	C	218	ARG	O-C-N	-9.28	107.86	122.70
1	B	218	ARG	O-C-N	-9.21	107.97	122.70
1	B	64	THR	O-C-N	-8.69	108.80	122.70
1	D	218	ARG	O-C-N	-8.66	108.84	122.70
1	C	64	THR	CA-C-N	8.33	135.53	117.20
1	A	170	GLY	O-C-N	-8.19	109.28	123.20
1	C	218	ARG	NE-CZ-NH2	8.15	124.38	120.30
1	B	255	GLU	CA-CB-CG	-7.78	96.28	113.40
1	A	255	GLU	N-CA-CB	-7.58	96.95	110.60
1	D	190	ALA	O-C-N	7.28	134.35	122.70
1	A	218	ARG	CA-C-N	7.28	133.21	117.20
1	B	218	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	A	218	ARG	NE-CZ-NH2	7.20	123.90	120.30
1	A	128	PRO	O-C-N	6.94	133.81	122.70
1	B	395	LYS	C-N-CA	-6.92	104.40	121.70
1	C	229	ASP	CA-C-N	-6.90	102.03	117.20
1	D	324	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	D	123	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	D	218	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	A	282	LYS	C-N-CA	6.60	138.19	121.70
1	B	255	GLU	N-CA-CB	6.55	122.40	110.60
1	D	218	ARG	CA-C-N	6.31	131.08	117.20
1	C	218	ARG	CA-C-N	6.17	130.78	117.20
1	D	62	MET	CG-SD-CE	6.15	110.04	100.20
1	C	215	MET	CG-SD-CE	6.14	110.03	100.20
1	D	165	MET	CG-SD-CE	6.14	110.02	100.20
1	A	215	MET	CG-SD-CE	6.13	110.01	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	MET	CG-SD-CE	6.11	109.98	100.20
1	B	62	MET	CG-SD-CE	6.11	109.98	100.20
1	B	215	MET	CG-SD-CE	6.09	109.94	100.20
1	D	215	MET	CG-SD-CE	6.04	109.86	100.20
1	B	64	THR	CA-C-N	6.02	130.44	117.20
1	D	124	MET	CG-SD-CE	5.94	109.71	100.20
1	A	282	LYS	O-C-N	-5.87	113.31	122.70
1	C	62	MET	CG-SD-CE	5.85	109.57	100.20
1	C	255	GLU	CA-CB-CG	5.83	126.22	113.40
1	B	177	PHE	N-CA-C	-5.82	95.28	111.00
1	A	238	LEU	O-C-N	-5.64	113.67	122.70
1	C	228	GLU	O-C-N	5.60	131.66	122.70
1	B	218	ARG	CA-C-N	5.60	129.51	117.20
1	A	128	PRO	CA-C-N	-5.51	105.09	117.20
1	A	63	ASN	O-C-N	5.50	131.50	122.70
1	D	326	THR	O-C-N	-5.50	113.90	122.70
1	D	191	ASN	O-C-N	5.44	131.41	122.70
1	A	226	VAL	O-C-N	-5.40	114.06	122.70
1	C	177	PHE	N-CA-C	-5.28	96.75	111.00
1	A	178	LEU	CA-CB-CG	5.16	127.16	115.30
1	D	177	PHE	N-CA-C	-5.06	97.33	111.00

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	2974	85	0
1	B	2990	0	2978	65	0
1	C	2990	0	2977	79	0
1	D	2990	0	2975	111	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	12028	315	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 13.

All (315) 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	1.43
1:D:256:ARG:HH11	1:D:256:ARG:HG3	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:CZ	1:A:284:PHE:CD1	2.43	0.94
1:B:374:ILE:HA	1:B:378:THR:HG22	1.50	0.90
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
1:A:152:GLU:HB2	1:A:159:ILE:HG23	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:256:ARG:HH11	1:D:256:ARG:CG	2.01	0.71
1:D:192:LYS:O	1:D:192:LYS:HD2	1.90	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: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: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:D:153:LYS:HE3	1:D:234:LYS:HD2	1.77	0.66
1:C:62:MET:SD	1:C:98:ILE:HG23	2.36	0.66
1:C:160:ILE:HG21	1:C:178:LEU:HD21	1.78	0.66
1:D:256:ARG:CD	3:D:2124:HOH:O	2.41	0.66
1:C:71:GLY:HA3	1:C:125:THR:HG21	1.78	0.66
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.60	0.65
1:A:370:LYS:HZ3	1:B:345:THR:HG22	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:C:103:LEU:C	1:C:103:LEU:HD22	2.18	0.63
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:D:300:GLU:O	1:D:304:LYS:HG3	1.99	0.62
1:A:309:ARG:O	1:A:313:GLN: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: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
1:B:294:ILE:HD13	1:B:297:MET:HE3	1.82	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:138:PRO:HD3	1:D:165:MET:HB2	1.84	0.58
1:A:134:CYS:HA	1:A:167:ILE:HD12	1.83	0.58
1:B:377:GLY:HA2	3:B:2048:HOH:O	2.02	0.58
1:A:149:THR:HG23	1:A:162:GLY:HA3	1.84	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:D:150:LYS:NZ	1:D:184:PRO:HG3	2.18	0.58
1:C:171:GLY:N	1:C:223:ARG:HD2	2.19	0.57
1:C:106:MET:O	1:C:110:ILE:HG12	2.04	0.57
1:D:268:GLN:NE2	1:D:309:ARG:HH22	2.01	0.57
1:B:294:ILE:HD13	1:B:297:MET:HE1	1.86	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:HD22	1:C:325:ASN:H	1.53	0.57
1:D:182:SER:O	1:D:184:PRO:HD3	2.04	0.57
1:C:154:LYS:HA	1:C:154:LYS:HE3	1.87	0.56
1:C:189:PRO:HG2	1:C:192:LYS:HG2	1.86	0.56
1:D:233:PRO:HD2	1:D:236:ASN:HD22	1.69	0.56
1:C:268:GLN:HE21	1:C:309:ARG:HH22	1.53	0.56
1:D:256:ARG:CG	1:D:256:ARG:NH1	2.63	0.56
1:D:153:LYS:HB2	1:D:158:TYR:CE2	2.41	0.56
1:A:132:ALA:HB3	1:A:176:TYR:HD1	1.70	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:B:341:ASN:HD21	1:B:370:LYS:HA	1.70	0.55
1:D:146:GLY:O	1:D:148:LYS:HD3	2.06	0.55
1:A:177:PHE:HE1	1:A:238:LEU:HD12	1.70	0.55
1:D:19:GLN:CD	1:D:19:GLN:H	2.08	0.55
1:A:255:GLU:O	1:A:258:VAL:HG13	2.07	0.55
1:A:106:MET:CE	1:A:254:LYS:HG2	2.37	0.54
1:A:215:MET:HB2	1:B:363:GLU:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:TRP:HA	1:D:200:GLU:HA	1.90	0.54
1:D:159:ILE:HD13	1:D:231:LYS:HE3	1.88	0.54
1:B:135:VAL:HG22	1:B:179:LEU:HB2	1.90	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:C:26:THR:HG22	1:C:61:LEU:HD11	1.89	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: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:D:17:THR:H	1:D:20:GLN:NE2	2.07	0.53
1:A:216:GLY:HA3	1:B:356:PHE:CZ	2.44	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:C:235:GLU:HG3	3:C:2227:HOH:O	2.09	0.52
1:A:292:GLN:HE21	1:D:384:LEU:HD21	1.74	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: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:A:255:GLU:OE1	1:A:255:GLU:HA	2.10	0.51
1:C:103:LEU:C	1:C:103:LEU:CD2	2.78	0.51
1:C:215:MET:HB2	1:D:363:GLU:CG	2.39	0.51
1:D:134:CYS:HB3	1:D:164:LYS:HG3	1.92	0.51
1:C:286:LYS:HD3	1:C:290:GLU:HB3	1.93	0.51
1:B:282:LYS:HD2	1:B:285:GLY:O	2.11	0.51
1:B:106:MET:HE2	1:B:110:ILE:HG23	1.91	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
1:D:64:THR:HB	1:D:75:LEU:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LYS:HB3	1:C:286:LYS:NZ	2.26	0.50
1:D:73:LEU:HB3	1:D:75:LEU:HD22	1.94	0.50
1:A:124:MET:N	1:A:124:MET:SD	2.83	0.50
1:C:366:MET:HB3	1:D:215:MET:HE3	1.93	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:D:161:ASN:HA	1:D:227:PHE:O	2.12	0.49
1:A:81:CYS:HB3	1:A:312:TYR:CE1	2.47	0.49
1:A:123:ARG:HH11	1:A:174:ASN:HD21	1.60	0.49
1:D:117:LYS:HA	1:D:121:LEU:HD23	1.94	0.48
1:C:17:THR:OG1	1:C:20:GLN:HG3	2.13	0.48
1:A:324:ARG:HH11	1:A:324:ARG:HB3	1.78	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:D:175:TRP:CE3	1:D:198:ILE:HD13	2.49	0.48
1:C:40:ALA:O	1:C:44:LYS:HG3	2.13	0.48
1:B:318:GLU:HB3	1:B:325:ASN:HB3	1.94	0.48
1:A:338:ASP:HA	1:A:373:GLN:HE21	1.77	0.48
1:A:66:ILE:HD13	1:A:121:LEU:O	2.13	0.48
1:C:171:GLY:HA3	1:C:208:ILE:HG21	1.95	0.48
1:B:355:GLY:O	1:B:363:GLU:HB2	2.13	0.48
1:D:371:ILE:HD13	1:D:375:TYR:CZ	2.48	0.48
1:D:153:LYS:CE	1:D:234:LYS:HD2	2.42	0.48
1:C:325:ASN:N	1:C:325:ASN:HD22	2.12	0.48
1:C:171:GLY:HA3	1:C:223:ARG:HD2	1.96	0.47
1:B:294:ILE:O	1:B:298:LEU:HG	2.14	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:HG21	1.95	0.47
1:D:197:PHE:CE2	1:D:237:VAL:HG22	2.48	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:A:296:PHE:O	1:A:300:GLU:HG3	2.15	0.47
1:C:48:TYR:CZ	1:C:172:LYS:HG2	2.48	0.47
1:A:95:GLN:O	1:A:99:GLU:HB2	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:LEU:HD21	1:D:391:ILE:HG23	1.97	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: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:C:269:ARG:HG3	1:C:365:LEU:HD21	1.98	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:CA	1:C:154:LYS:HE3	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:D:150:LYS:HZ2	1:D:184:PRO:HG3	1.80	0.46
1:C:267:ALA:HB1	1:C:343:LEU:HD22	1.96	0.46
1:B:161:ASN:HA	1:B:227:PHE:O	2.16	0.46
1:A:207:GLN:HB2	1:A:226:VAL:HB	1.97	0.46
1:C:189:PRO:HG2	1:C:192:LYS:CG	2.46	0.46
1:C:17:THR:H	1:C:20:GLN:HE21	1.63	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:C:171:GLY:CA	1:C:223:ARG:HD2	2.46	0.45
1:A:106:MET:HE2	1:A:254:LYS:HG2	1.98	0.45
1:B:381:ILE:O	1:B:385:ILE:HG13	2.15	0.45
1:B:277:TYR:CE2	1:B:281:ARG:HG3	2.51	0.45
1:A:103:LEU:HD13	1:A:133:TYR:CB	2.46	0.45
1:D:382:GLN:O	1:D:386:VAL:HG23	2.16	0.45
1:C:168:THR:O	1:C:169:ASN:HB2	2.16	0.45
1:D:169:ASN:HD22	1:D:169:ASN:N	2.15	0.45
1:A:17:THR:O	1:A:21:LYS:HG3	2.16	0.45
1:C:67:PRO:HD2	1:C:121:LEU:HD23	1.98	0.45
1:A:294:ILE:HD11	2:B:399:FAD:H1B	1.99	0.45
1:B:384:LEU:HD21	1:C:292:GLN:HE21	1.82	0.45
1:D:296:PHE:O	1:D:300:GLU:HG3	2.17	0.45
1:D:238:LEU:HA	1:D:238:LEU:HD13	1.78	0.45
1:D:207:GLN:HG3	1:D:226:VAL:HB	1.99	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:B:315:ALA:O	1:B:319:VAL:HG23	2.17	0.45
1:D:108:ILE:HG22	1:D:121:LEU:HD21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:385:ILE:O	1:D:389:GLU:HG2	2.15	0.45
1:C:268:GLN:NE2	1:C:309:ARG:HH22	2.14	0.44
1:C:387:ALA:O	1:C:391:ILE:HG12	2.17	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: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:D:48:TYR:CD1	1:D:49:PRO:HD2	2.53	0.44
1:A:177:PHE:CE1	1:A:238:LEU:HD12	2.52	0.44
1:A:299:ALA:O	1:A:303:MET:HG3	2.18	0.44
1:A:184:PRO:O	1:A:186:PRO:HD3	2.18	0.44
1:D:36:ILE:HG12	1:D:269:ARG:HH21	1.81	0.44
1:B:319:VAL:HG22	1:B:325:ASN:CG	2.37	0.44
1:A:210:ARG:HG3	1:A:211:LYS:N	2.32	0.44
1:D:99:GLU:OE1	1:D:99:GLU:HA	2.18	0.43
1:B:296:PHE:HE1	1:C:384:LEU:HD13	1.83	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:159:ILE:HD11	1:D:229:ASP:HA	1.99	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:A:137:GLU:HB3	1:A:163:GLN:O	2.18	0.43
1:D:228:GLU:O	1:D:229:ASP:HB2	2.18	0.43
1:C:203:THR:CG2	1:C:204:PRO:HD2	2.48	0.43
1:D:85:GLU:OE2	1:D:309:ARG:HD3	2.18	0.43
1:C:112:GLY:O	1:C:117:LYS:HE3	2.17	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: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
1:D:216:GLY:C	1:D:218:ARG:N	2.72	0.43
1:D:50:VAL:HB	1:D:51:PRO:HD3	2.00	0.43
1:D:213:LEU:N	1:D:213:LEU:CD2	2.80	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: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:C:165:MET:HG3	1:C:166:TRP:CD1	2.54	0.42
1:A:301:MET:O	1:A:305:VAL:HG23	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:O	1:A:345:THR:HG22	2.18	0.42
1:D:249:MET:O	1:D:253:ASP:HB2	2.20	0.42
1:D:185:ASP:HA	1:D:186:PRO:HD2	1.82	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:A:134:CYS:HB3	1:A:164:LYS:HG3	2.00	0.42
1:C:378:THR:O	1:C:382:GLN:HG2	2.19	0.42
1:A:236:ASN:HD22	1:A:236:ASN:HA	1.65	0.42
1:D:260:ALA:CA	1:D:261:ALA:N	2.72	0.42
1:B:171:GLY:HA2	1:B:208:ILE:HD13	2.02	0.42
1:C:103:LEU:HA	1:C:103:LEU:HD23	1.60	0.42
1:D:281:ARG:HB3	1:D:288:LEU:HD22	2.00	0.42
1:A:267:ALA:HB1	1:A:343:LEU:HD22	2.00	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:D:106:MET:HA	1:D:106:MET:HE3	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:N	1:C:115:GLN:OE1	2.53	0.42
1:C:154:LYS:HD2	1:C:159:ILE:CD1	2.50	0.42
1:B:147:ILE:HD11	1:B:179:LEU:HD13	2.00	0.42
1:C:149:THR:HG23	1:C:162:GLY:HA3	2.02	0.42
1:B:267:ALA:HB1	1:B:343:LEU:HD22	2.00	0.42
1:B:268:GLN:NE2	1:B:309:ARG:HH22	2.06	0.41
1:A:286:LYS:HB2	1:A:291:HIS:CE1	2.55	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:D:156:ASP:O	1:D:234:LYS:HB2	2.20	0.41
1:C:142:SER:HB3	1:C:381:ILE:HG21	2.02	0.41
1:D:113:ASN:OD1	1:D:115:GLN:HB3	2.20	0.41
1:B:165:MET:HG3	1:B:166:TRP:CD1	2.55	0.41
1:A:101:ASN:OD1	1:A:130:MET:HA	2.21	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: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:A:312:TYR:CD1	1:A:312:TYR:C	2.94	0.41
1:D:378:THR:O	1:D:382:GLN:HG2	2.20	0.41
1:D:362:VAL:HA	1:D:365:LEU:HD12	2.02	0.41
1:B:283:THR:O	1:B:284:PHE:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.56	0.41
1:D:377:GLY:HA3	1:D:382:GLN:HE21	1.85	0.40
1:A:23:PHE:CE2	1:A:75:LEU:HD21	2.57	0.40
1:B:368:ASP:O	1:B:371:ILE:HD11	2.21	0.40
1:C:366:MET:HB3	1:D:215:MET:CE	2.51	0.40
1:B:120:TYR:CD1	1:B:198:ILE:HD11	2.57	0.40
1:D:377:GLY:HA3	1:D:382:GLN:NE2	2.37	0.40
1:D:101:ASN:HA	1:D:131:CYS:SG	2.62	0.40
1:B:256:ARG:NE	1:B:382:GLN:HE22	2.19	0.40
1:C:136:THR:CG2	1:C:137:GLU:N	2.83	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:A:144:VAL:O	1:A:147:ILE:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	385/396 (97%)	357 (93%)	26 (7%)	2 (0%)	34	48
1	B	385/396 (97%)	370 (96%)	15 (4%)	0	100	100
1	C	385/396 (97%)	370 (96%)	13 (3%)	2 (0%)	34	48
1	D	385/396 (97%)	355 (92%)	28 (7%)	2 (0%)	34	48
All	All	1540/1584 (97%)	1452 (94%)	82 (5%)	6 (0%)	39	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	THR
1	D	166	TRP

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Mol	Chain	Res	Type
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%)	285 (94%)	18 (6%)	24	38
1	B	303/310 (98%)	282 (93%)	21 (7%)	19	30
1	C	303/310 (98%)	279 (92%)	24 (8%)	15	23
1	D	303/310 (98%)	271 (89%)	32 (11%)	8	12
All	All	1212/1240 (98%)	1117 (92%)	95 (8%)	16	24

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	99	GLU
1	A	103	LEU
1	A	137	GLU
1	A	156	ASP
1	A	159	ILE
1	A	192	LYS
1	A	228	GLU
1	A	236	ASN
1	A	249	MET
1	A	258	VAL
1	A	298	LEU
1	A	312	TYR
1	A	319	VAL
1	A	324	ARG
1	A	333	LYS
1	A	365	LEU

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Mol	Chain	Res	Type
1	A	375	TYR
1	B	10	LEU
1	B	75	LEU
1	B	115	GLN
1	B	121	LEU
1	B	163	GLN
1	B	179	LEU
1	B	191	ASN
1	B	198	ILE
1	B	199	VAL
1	B	210	ARG
1	B	217	GLN
1	B	271	LEU
1	B	279	LEU
1	B	281	ARG
1	B	307	LEU
1	B	314	ARG
1	B	319	VAL
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	142	SER
1	C	152	GLU
1	C	154	LYS
1	C	179	LEU
1	C	192	LYS
1	C	210	ARG
1	C	238	LEU
1	C	255	GLU
1	C	286	LYS
1	C	290	GLU
1	C	295	SER
1	C	298	LEU
1	C	307	LEU
1	C	312	TYR
1	C	325	ASN
1	C	348	VAL
1	C	358	THR

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Mol	Chain	Res	Type
1	C	365	LEU
1	C	371	ILE
1	C	375	TYR
1	C	396	ASN
1	D	19	GLN
1	D	29	LYS
1	D	47	GLU
1	D	48	TYR
1	D	55	ARG
1	D	58	GLU
1	D	75	LEU
1	D	85	GLU
1	D	95	GLN
1	D	156	ASP
1	D	165	MET
1	D	178	LEU
1	D	191	ASN
1	D	198	ILE
1	D	199	VAL
1	D	207	GLN
1	D	246	LYS
1	D	253	ASP
1	D	256	ARG
1	D	269	ARG
1	D	282	LYS
1	D	288	LEU
1	D	295	SER
1	D	312	TYR
1	D	314	ARG
1	D	319	VAL
1	D	324	ARG
1	D	325	ASN
1	D	343	LEU
1	D	375	TYR
1	D	392	ASP
1	D	396	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	ASN
1	A	207	GLN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	341	ASN
1	A	342	GLN
1	B	65	HIS
1	B	105	GLN
1	B	268	GLN
1	B	341	ASN
1	B	373	GLN
1	C	20	GLN
1	C	63	ASN
1	C	69	ASN
1	C	95	GLN
1	C	116	GLN
1	C	169	ASN
1	C	268	GLN
1	C	313	GLN
1	C	325	ASN
1	C	373	GLN
1	C	382	GLN
1	D	20	GLN
1	D	95	GLN
1	D	115	GLN
1	D	169	ASN
1	D	174	ASN
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 carbohydrates 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	-	48,58,58	1.37	6 (12%)	54,89,89	2.90	13 (24%)
2	FAD	B	399	-	48,58,58	1.36	6 (12%)	54,89,89	2.96	15 (27%)
2	FAD	C	399	-	48,58,58	1.41	6 (12%)	54,89,89	2.63	13 (24%)
2	FAD	D	399	-	48,58,58	1.58	11 (22%)	54,89,89	2.73	10 (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	-	-	0/30/50/50	0/6/6/6
2	FAD	B	399	-	-	0/30/50/50	0/6/6/6
2	FAD	C	399	-	-	0/30/50/50	0/6/6/6
2	FAD	D	399	-	-	0/30/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	399	FAD	C1'-N10	-3.03	1.45	1.48
2	A	399	FAD	C8A-N7A	-2.59	1.29	1.34
2	A	399	FAD	C1'-N10	-2.59	1.45	1.48
2	B	399	FAD	C5A-C4A	-2.35	1.35	1.40
2	D	399	FAD	P-O2P	-2.18	1.45	1.54
2	D	399	FAD	C8A-N7A	-2.11	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	399	FAD	C5A-C4A	-2.06	1.35	1.40
2	D	399	FAD	C1'-N10	-2.06	1.46	1.48
2	D	399	FAD	PA-O2A	-2.04	1.46	1.54
2	C	399	FAD	PA-O2A	-2.01	1.46	1.54
2	B	399	FAD	C4X-N5	2.01	1.36	1.33
2	C	399	FAD	C4-N3	2.13	1.37	1.33
2	C	399	FAD	C9A-N10	2.14	1.41	1.38
2	D	399	FAD	C9A-N10	2.41	1.42	1.38
2	A	399	FAD	C4-N3	2.72	1.38	1.33
2	B	399	FAD	C4-N3	2.74	1.38	1.33
2	C	399	FAD	C4X-N5	2.76	1.37	1.33
2	B	399	FAD	C9A-N10	2.78	1.42	1.38
2	D	399	FAD	C4X-N5	3.10	1.38	1.33
2	C	399	FAD	C4-C4X	3.19	1.47	1.41
2	D	399	FAD	C4-N3	3.21	1.39	1.33
2	D	399	FAD	C4-C4X	3.21	1.47	1.41
2	A	399	FAD	C4-C4X	3.24	1.47	1.41
2	D	399	FAD	O4B-C1B	3.27	1.45	1.41
2	A	399	FAD	C4X-N5	3.42	1.38	1.33
2	A	399	FAD	O4B-C1B	4.09	1.46	1.41
2	B	399	FAD	C10-N10	4.39	1.44	1.39
2	D	399	FAD	C10-N10	4.78	1.44	1.39
2	C	399	FAD	C10-N10	5.60	1.45	1.39

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	399	FAD	C4X-C10-N10	-7.84	115.90	120.52
2	D	399	FAD	C4X-C10-N10	-7.11	116.33	120.52
2	A	399	FAD	C4X-C4-N3	-6.96	114.08	123.59
2	C	399	FAD	C4X-C10-N10	-6.93	116.43	120.52
2	D	399	FAD	C4-C4X-C10	-6.57	115.74	119.94
2	D	399	FAD	C4X-C4-N3	-6.50	114.70	123.59
2	C	399	FAD	C4X-C4-N3	-6.12	115.23	123.59
2	A	399	FAD	C4X-C10-N10	-6.11	116.92	120.52
2	B	399	FAD	C4X-C4-N3	-6.09	115.26	123.59
2	A	399	FAD	C2B-C1B-N9A	-5.94	105.22	114.29
2	A	399	FAD	C4-C4X-C10	-5.41	116.48	119.94
2	B	399	FAD	C4-C4X-C10	-4.75	116.90	119.94
2	A	399	FAD	C4X-N5-C5X	-3.87	112.31	116.76
2	B	399	FAD	C2B-C1B-N9A	-3.69	108.65	114.29
2	C	399	FAD	C4-C4X-C10	-3.68	117.59	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	399	FAD	C4X-N5-C5X	-3.43	112.81	116.76
2	C	399	FAD	C2B-C1B-N9A	-3.34	109.19	114.29
2	D	399	FAD	C2B-C1B-N9A	-3.33	109.21	114.29
2	C	399	FAD	C4X-N5-C5X	-3.31	112.96	116.76
2	C	399	FAD	C6-C5X-N5	-3.30	114.72	118.96
2	C	399	FAD	O3P-P-O5'	-3.25	94.31	102.94
2	A	399	FAD	P-O3P-PA	-3.22	123.70	132.73
2	B	399	FAD	O4'-C4'-C3'	-3.21	100.95	109.02
2	B	399	FAD	C4-C4X-N5	-3.11	114.95	118.72
2	B	399	FAD	O3'-C3'-C4'	-3.07	101.01	108.75
2	B	399	FAD	O3P-P-O5'	-2.86	95.36	102.94
2	D	399	FAD	C4X-N5-C5X	-2.82	113.52	116.76
2	B	399	FAD	C6-C5X-N5	-2.76	115.41	118.96
2	B	399	FAD	C2B-C3B-C4B	-2.74	96.97	102.61
2	C	399	FAD	C4-C4X-N5	-2.70	115.44	118.72
2	C	399	FAD	O2'-C2'-C1'	-2.60	103.56	109.94
2	D	399	FAD	O3B-C3B-C2B	-2.58	103.43	111.83
2	D	399	FAD	C6-C5X-N5	-2.41	115.86	118.96
2	C	399	FAD	C1'-N10-C9A	-2.22	116.37	118.86
2	A	399	FAD	C6-C5X-N5	-2.22	116.11	118.96
2	B	399	FAD	N3A-C2A-N1A	-2.20	127.21	128.89
2	D	399	FAD	O3P-PA-O5B	2.08	108.44	102.94
2	B	399	FAD	O4B-C1B-N9A	2.09	112.48	108.10
2	A	399	FAD	O4B-C1B-N9A	2.14	112.57	108.10
2	C	399	FAD	O5B-C5B-C4B	2.53	118.46	109.12
2	A	399	FAD	O4'-C4'-C3'	2.55	115.43	109.02
2	A	399	FAD	C9A-C5X-N5	2.73	126.40	122.36
2	A	399	FAD	O5B-C5B-C4B	2.78	119.39	109.12
2	A	399	FAD	C4A-C5A-N7A	3.14	112.37	109.48
2	B	399	FAD	C9A-C5X-N5	3.23	127.13	122.36
2	D	399	FAD	C9A-C5X-N5	3.24	127.14	122.36
2	C	399	FAD	C9A-C5X-N5	3.70	127.83	122.36
2	C	399	FAD	C4-N3-C2	12.47	126.02	115.25
2	D	399	FAD	C4-N3-C2	13.43	126.85	115.25
2	A	399	FAD	C4-N3-C2	13.84	127.21	115.25
2	B	399	FAD	C4-N3-C2	14.88	128.11	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.