



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 07:55 pm BST

PDB ID : 2EBA
Title : Crystal structure of the putative glutaryl-CoA dehydrogenase from thermus thermophilus
Authors : Kumarevel, T.S.; Karthe, P.; Kuramitsu, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-07
Resolution : 2.21 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

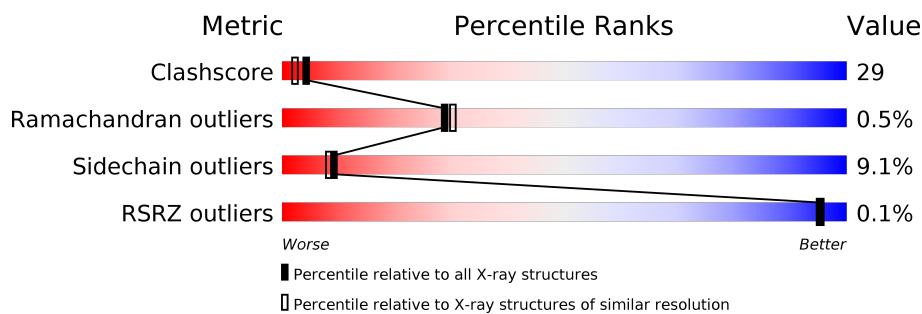
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.21 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	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	385	<div> <div>61%</div> <div>32%</div> <div>5%</div> </div>
1	C	385	<div> <div>54%</div> <div>39%</div> <div>6%</div> </div>
1	D	385	<div> <div>55%</div> <div>37%</div> <div>6%</div> </div>
1	E	385	<div> <div>54%</div> <div>39%</div> <div>5%</div> </div>
1	F	385	<div> <div>56%</div> <div>36%</div> <div>6%</div> </div>
1	G	385	<div> <div>58%</div> <div>32%</div> <div>8%</div> </div>
1	H	385	<div> <div>60%</div> <div>34%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	I	385	 A horizontal bar chart showing the quality of chain I. The bar is divided into three segments: green (59%), yellow (34%), and orange (5%). The segments are labeled with their respective percentages: 59%, 34%, and 5%.

2 Entry composition

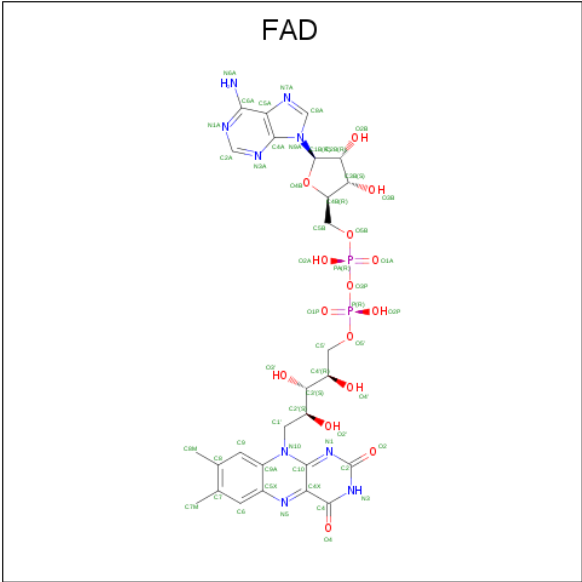
There are 3 unique types of molecules in this entry. The entry contains 24912 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative glutaryl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	C	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	D	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	E	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	F	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	G	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	H	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			
1	I	380	Total	C	N	O	S	0	0	0
			2986	1915	517	541	13			

- 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	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	I	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	87	Total	O	0	0
			87	87		
3	C	77	Total	O	0	0
			77	77		
3	D	71	Total	O	0	0
			71	71		
3	E	71	Total	O	0	0
			71	71		

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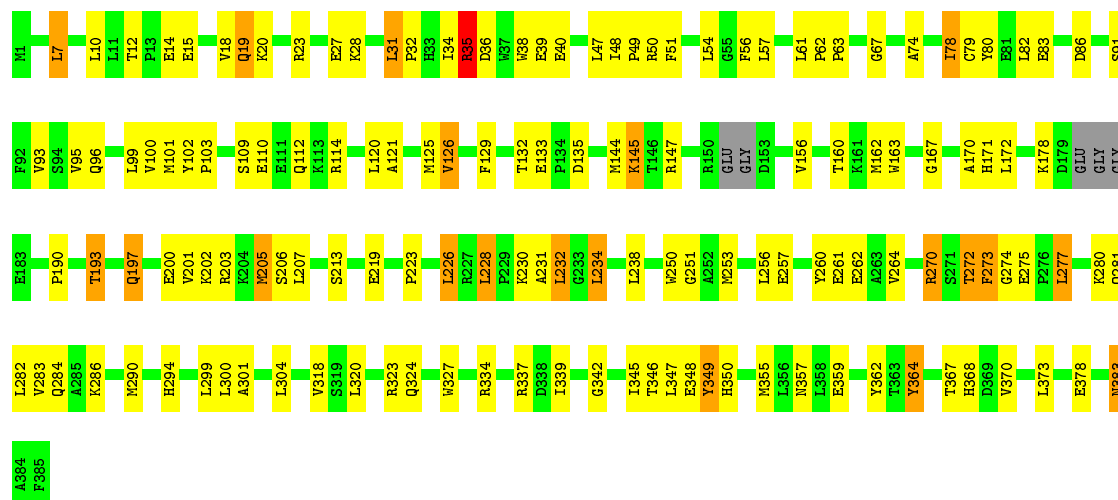
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	55	Total 55	O 55	0	0
3	G	83	Total 83	O 83	0	0
3	H	84	Total 84	O 84	0	0
3	I	72	Total 72	O 72	0	0

3 Residue-property plots

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

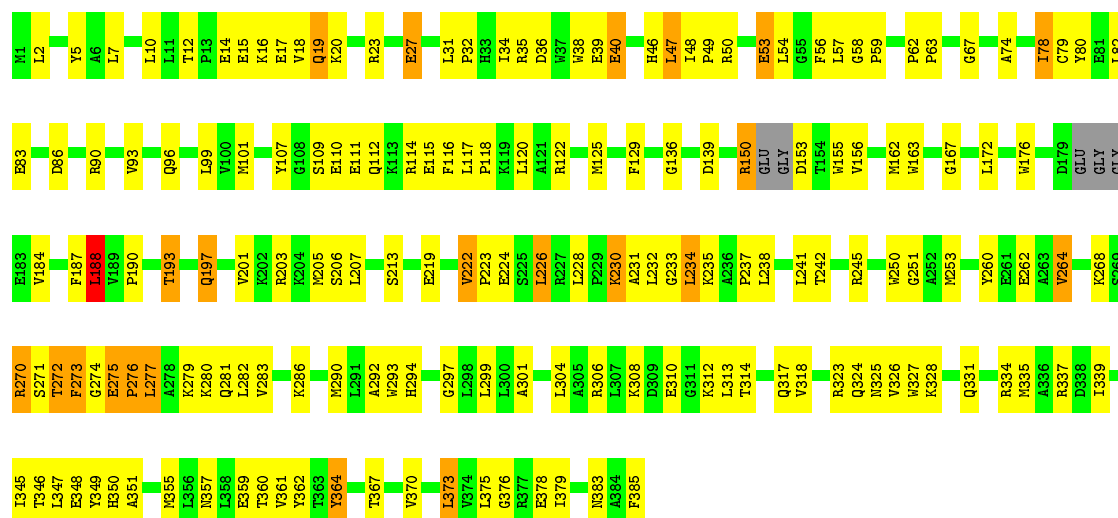
• Molecule 1: Putative glutaryl-CoA dehydrogenase

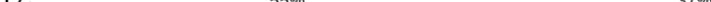
Chain A: 

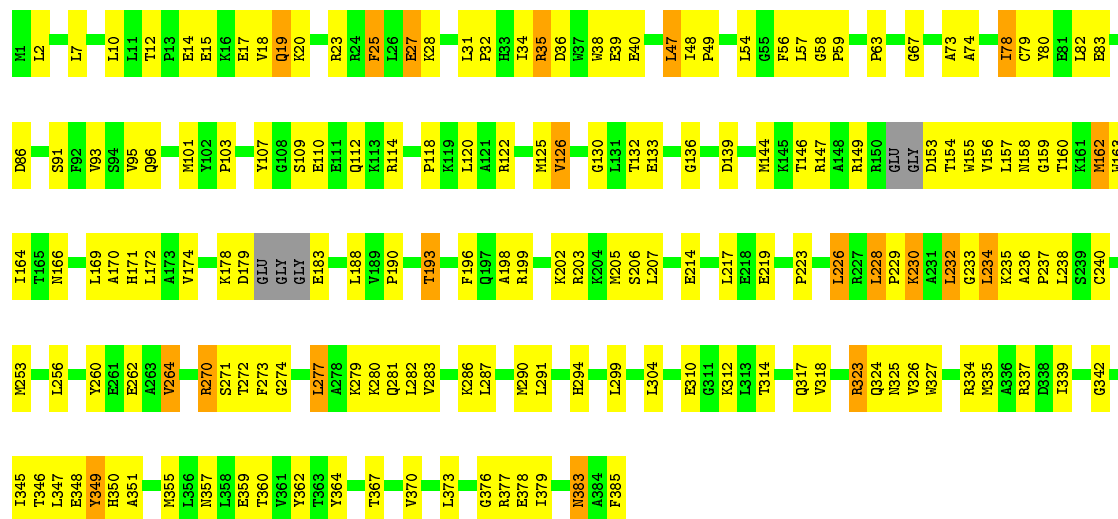


• Molecule 1: Putative glutaryl-CoA dehydrogenase

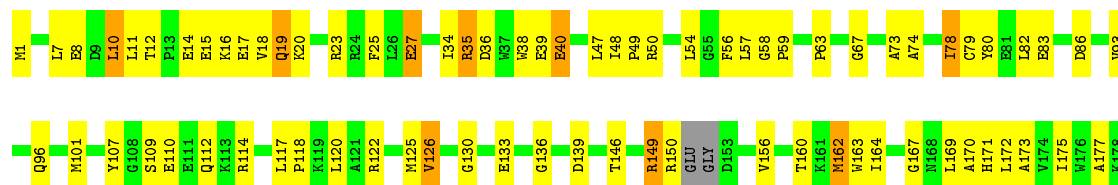
Chain C: 

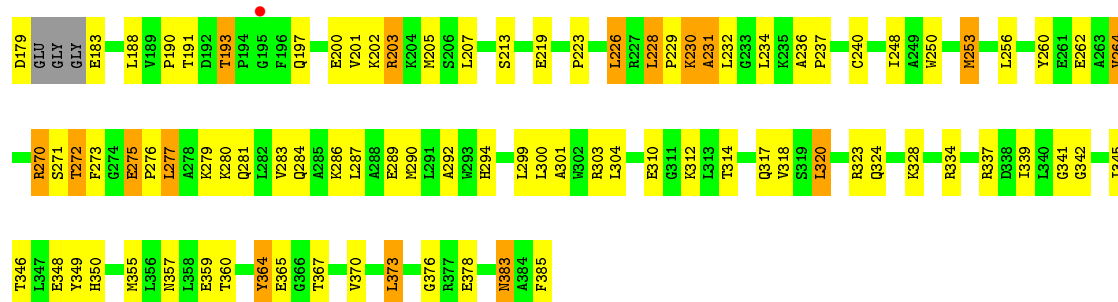


Chain D:  55% 37% 6%



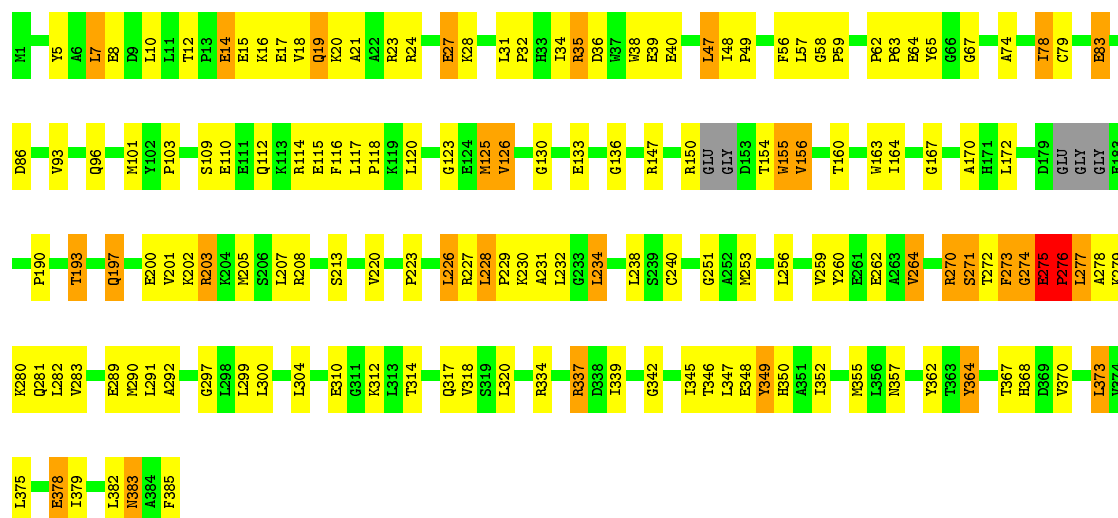
Chain F: 56% 36% 6%





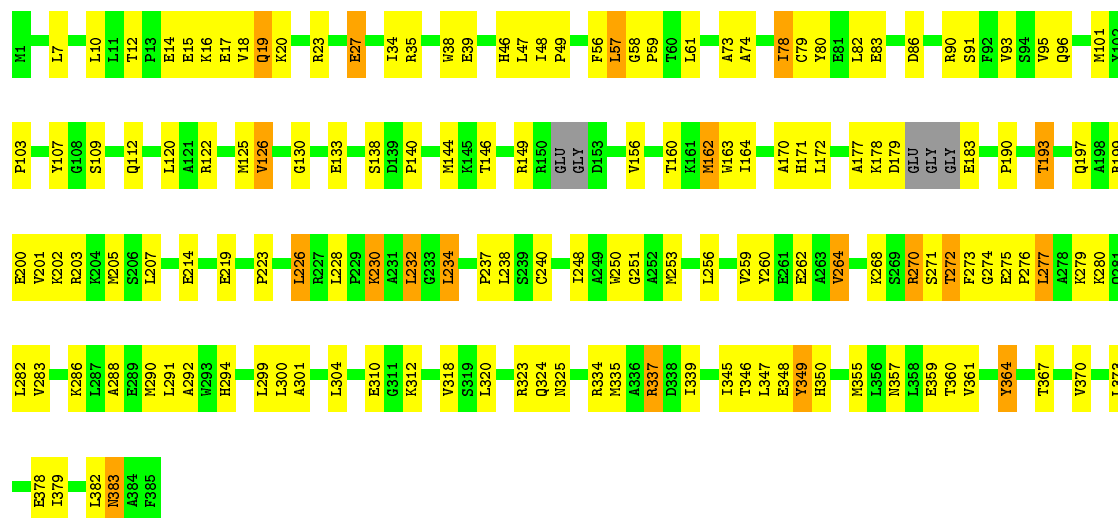
- Molecule 1: Putative glutaryl-CoA dehydrogenase

Chain G: 58% 32% 8% ..



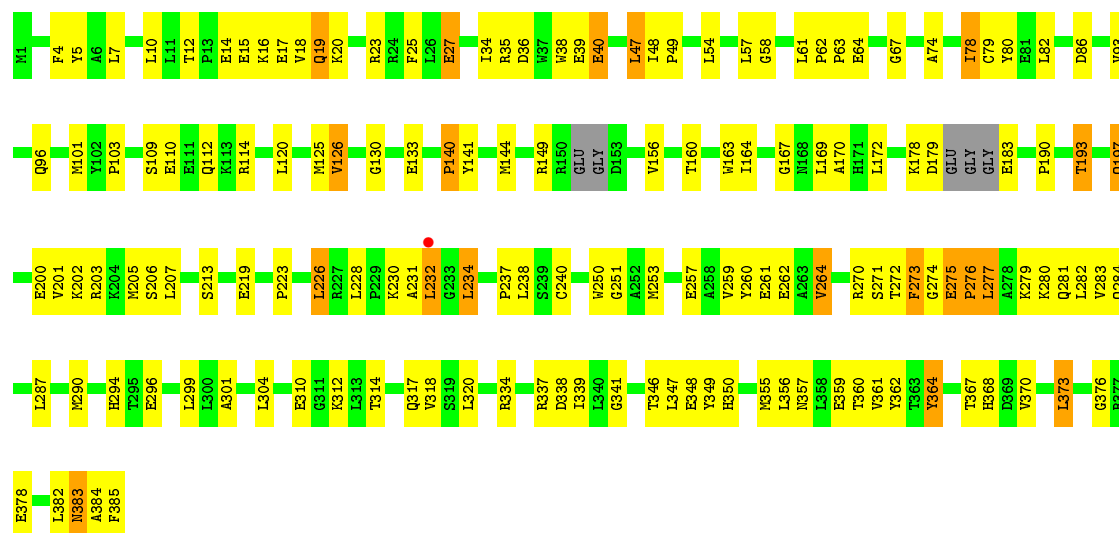
- Molecule 1: Putative glutaryl-CoA dehydrogenase

Chain H: 60% 34% 5% ..



- Molecule 1: Putative glutaryl-CoA dehydrogenase

Chain I:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.24Å 86.24Å 157.42Å 75.92° 81.25° 64.24°	Depositor
Resolution (Å)	19.96 – 2.21 40.19 – 2.21	Depositor EDS
% Data completeness (in resolution range)	72.8 (19.96-2.21) 72.9 (40.19-2.21)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 2.22Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.260 , 0.275 0.259 , (Not available)	Depositor DCC
R_{free} test set	891 reflections (0.68%)	wwPDB-VP
Wilson B-factor (Å ²)	14.6	Xtriage
Anisotropy	0.612	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 21.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	24912	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.51	1/3053 (0.0%)	0.72	3/4131 (0.1%)
1	C	0.56	0/3053	0.79	2/4131 (0.0%)
1	D	0.51	0/3053	0.77	3/4131 (0.1%)
1	E	0.52	0/3053	0.77	5/4131 (0.1%)
1	F	0.46	0/3053	0.70	1/4131 (0.0%)
1	G	0.57	3/3053 (0.1%)	0.72	4/4131 (0.1%)
1	H	0.44	0/3053	0.69	2/4131 (0.0%)
1	I	0.40	0/3053	0.64	1/4131 (0.0%)
All	All	0.50	4/24424 (0.0%)	0.73	21/33048 (0.1%)

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	G	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	155	TRP	CB-CG	-14.56	1.24	1.50
1	G	155	TRP	CD1-NE1	-8.99	1.22	1.38
1	A	274	GLY	CA-C	-5.21	1.43	1.51
1	G	155	TRP	CE3-CZ3	-5.13	1.29	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	275	GLU	N-CA-C	-9.85	84.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	274	GLY	N-CA-C	8.46	134.26	113.10
1	D	31	LEU	CA-CB-CG	-7.81	97.34	115.30
1	H	61	LEU	CB-CG-CD1	-6.98	99.13	111.00
1	E	153	ASP	C-N-CA	-6.94	104.35	121.70
1	F	275	GLU	C-N-CD	6.70	142.48	128.40
1	E	2	LEU	N-CA-C	-6.68	92.97	111.00
1	E	154	THR	N-CA-CB	6.43	122.51	110.30
1	G	274	GLY	N-CA-C	6.40	129.10	113.10
1	D	172	LEU	CA-CB-CG	-6.37	100.66	115.30
1	G	276	PRO	N-CA-C	-6.13	96.15	112.10
1	D	276	PRO	N-CA-C	-6.03	96.43	112.10
1	I	275	GLU	N-CA-C	-5.95	94.92	111.00
1	A	273	PHE	CA-C-N	-5.89	104.42	116.20
1	G	349	TYR	N-CA-C	5.50	125.85	111.00
1	C	272	THR	N-CA-C	5.49	125.81	111.00
1	E	349	TYR	N-CA-C	5.36	125.48	111.00
1	E	170	ALA	N-CA-C	5.30	125.30	111.00
1	A	349	TYR	N-CA-C	5.23	125.12	111.00
1	H	349	TYR	N-CA-C	5.15	124.90	111.00
1	C	188	LEU	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	154	THR	Mainchain

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	2986	0	3010	162	0
1	C	2986	0	3010	213	1
1	D	2986	0	3010	204	0
1	E	2986	0	3010	206	0
1	F	2986	0	3010	195	0
1	G	2986	0	3010	198	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2986	0	3010	199	0
1	I	2986	0	3010	207	1
2	A	53	0	31	4	0
2	C	53	0	31	5	0
2	D	53	0	31	5	0
2	E	53	0	31	3	0
2	F	53	0	31	2	0
2	G	53	0	31	1	0
2	H	53	0	31	1	0
2	I	53	0	31	4	0
3	A	87	0	0	3	0
3	C	77	0	0	4	0
3	D	71	0	0	8	0
3	E	71	0	0	10	1
3	F	55	0	0	4	0
3	G	83	0	0	11	0
3	H	84	0	0	14	0
3	I	72	0	0	8	0
All	All	24912	0	24328	1423	2

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 29.

All (1423) 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:C:253:MET:CE	1:C:294:HIS:HA	1.60	1.31
1:A:253:MET:CE	1:A:294:HIS:HA	1.72	1.20
1:F:253:MET:CE	1:F:294:HIS:HA	1.74	1.15
1:F:203:ARG:CD	1:G:35:ARG:HH21	1.59	1.15
1:A:19:GLN:NE2	1:A:20:LYS:HE2	1.62	1.15
1:H:253:MET:CE	1:H:294:HIS:HA	1.77	1.14
1:F:57:LEU:HB3	1:F:101:MET:HE1	1.30	1.13
1:C:272:THR:HG23	1:E:139:ASP:HB2	1.30	1.12
1:E:272:THR:HG22	1:E:273:PHE:N	1.61	1.12
1:I:253:MET:CE	1:I:294:HIS:HA	1.80	1.12
1:E:253:MET:HE1	1:E:294:HIS:HA	1.13	1.11
1:C:120:LEU:HD23	1:C:125:MET:O	1.47	1.11
1:C:35:ARG:HD2	1:E:203:ARG:CZ	1.81	1.10
1:G:36:ASP:O	1:G:40:GLU:HG3	1.49	1.10
1:E:35:ARG:O	1:E:39:GLU:HG3	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:MET:CE	1:D:294:HIS:HA	1.83	1.09
1:D:253:MET:HE1	1:D:294:HIS:HA	1.29	1.09
1:A:253:MET:HE1	1:A:294:HIS:HA	1.09	1.08
1:F:139:ASP:HB2	1:G:272:THR:HG23	1.34	1.08
1:I:272:THR:HG22	1:I:273:PHE:H	0.97	1.07
1:F:203:ARG:HD3	1:G:35:ARG:NH2	1.69	1.07
1:E:253:MET:CE	1:E:294:HIS:HA	1.83	1.07
1:E:162:MET:HE2	1:E:163:TRP:H	1.20	1.07
1:I:253:MET:HE1	1:I:294:HIS:HA	1.11	1.06
1:I:140:PRO:HD2	3:I:8031:HOH:O	1.54	1.05
1:A:19:GLN:HE22	1:A:20:LYS:HE2	1.08	1.04
1:C:187:PHE:O	1:C:188:LEU:HG	1.56	1.04
1:D:36:ASP:O	1:D:40:GLU:HG3	1.56	1.03
1:C:253:MET:HE1	1:C:294:HIS:CA	1.87	1.03
1:F:253:MET:HE1	1:F:294:HIS:HA	1.32	1.03
1:H:253:MET:HE1	1:H:294:HIS:HA	1.35	1.02
1:D:272:THR:HG22	1:D:273:PHE:CD1	1.94	1.02
1:A:19:GLN:HE22	1:A:20:LYS:CE	1.72	1.01
1:I:272:THR:HG22	1:I:273:PHE:N	1.73	1.01
1:F:203:ARG:HD3	1:G:35:ARG:HH21	0.86	1.00
1:E:57:LEU:HB3	1:E:101:MET:HE1	1.40	1.00
1:E:272:THR:HG22	1:E:273:PHE:H	1.18	0.99
1:D:162:MET:HE2	1:D:163:TRP:H	1.28	0.99
1:C:35:ARG:HD2	1:E:203:ARG:NH1	1.75	0.99
1:F:271:SER:HB2	1:F:275:GLU:O	1.63	0.99
1:G:272:THR:HG22	1:G:273:PHE:N	1.76	0.99
1:G:57:LEU:HB3	1:G:101:MET:HE1	1.45	0.98
1:C:275:GLU:CG	1:C:280:LYS:NZ	2.27	0.97
1:A:101:MET:HE1	1:A:121:ALA:HA	1.41	0.97
1:D:133:GLU:HG2	1:D:160:THR:O	1.64	0.97
1:H:272:THR:HG22	1:H:273:PHE:N	1.76	0.97
1:H:348:GLU:HB2	1:I:203:ARG:HH21	1.27	0.96
1:C:272:THR:HG22	1:C:273:PHE:N	1.79	0.96
1:D:272:THR:HG22	1:D:273:PHE:N	1.81	0.96
1:C:275:GLU:HG2	1:C:280:LYS:NZ	1.79	0.96
1:E:272:THR:HG22	1:E:273:PHE:CD1	2.01	0.96
1:H:183:GLU:OE1	1:H:232:LEU:HD11	1.66	0.96
1:G:272:THR:C	1:G:274:GLY:H	1.68	0.95
1:C:275:GLU:HG2	1:C:280:LYS:HZ1	1.28	0.94
1:I:272:THR:HG22	1:I:273:PHE:HD1	1.33	0.94
1:C:139:ASP:HB2	1:E:272:THR:HG23	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:19:GLN:NE2	1:G:20:LYS:HE3	1.83	0.93
1:C:253:MET:HE1	1:C:294:HIS:HA	0.94	0.93
1:D:162:MET:CE	1:D:163:TRP:H	1.82	0.93
1:C:58:GLY:HA3	1:C:101:MET:SD	2.09	0.91
1:H:125:MET:HE1	1:H:172:LEU:HD22	1.50	0.91
1:C:57:LEU:HB3	1:C:101:MET:HE1	1.51	0.91
1:C:277:LEU:O	1:C:283:VAL:HG21	1.70	0.90
1:I:96:GLN:O	1:I:101:MET:HG3	1.70	0.90
1:F:120:LEU:HD23	1:F:125:MET:O	1.71	0.90
1:E:272:THR:CG2	1:E:273:PHE:CD1	2.55	0.89
1:D:272:THR:HG22	1:D:273:PHE:HD1	1.33	0.89
1:C:271:SER:HB2	1:C:276:PRO:HA	1.53	0.89
1:D:162:MET:HE2	1:D:163:TRP:N	1.87	0.89
1:C:12:THR:OG1	1:C:15:GLU:HG3	1.73	0.88
1:I:57:LEU:C	1:I:101:MET:HE1	1.94	0.88
1:F:57:LEU:HB3	1:F:101:MET:CE	2.04	0.88
1:A:334:ARG:HA	1:A:355:MET:HE2	1.53	0.87
1:H:272:THR:HG22	1:H:273:PHE:H	1.35	0.87
1:E:96:GLN:O	1:E:101:MET:HG3	1.75	0.87
1:F:320:LEU:HD23	1:I:4:PHE:CE2	2.10	0.87
1:I:272:THR:HG22	1:I:273:PHE:CD1	2.09	0.86
1:I:277:LEU:O	1:I:283:VAL:HG21	1.74	0.86
1:C:35:ARG:HD2	1:E:203:ARG:NH2	1.90	0.85
1:G:334:ARG:HA	1:G:355:MET:HE2	1.58	0.85
1:D:162:MET:HE3	1:D:162:MET:HA	1.58	0.85
1:F:149:ARG:CZ	1:F:156:VAL:HG11	2.06	0.85
1:E:35:ARG:HD3	3:E:4002:HOH:O	1.75	0.85
1:D:272:THR:CG2	1:D:273:PHE:CD1	2.61	0.84
1:C:346:THR:HG22	1:C:348:GLU:H	1.43	0.84
1:H:96:GLN:O	1:H:101:MET:HG3	1.78	0.84
1:C:272:THR:HG22	1:C:273:PHE:CD1	2.12	0.83
1:D:346:THR:HG22	1:D:348:GLU:H	1.40	0.83
1:C:234:LEU:HD22	1:C:238:LEU:HG	1.59	0.83
1:E:35:ARG:HG3	1:E:35:ARG:HH11	1.42	0.83
1:I:272:THR:CG2	1:I:273:PHE:CD1	2.61	0.83
1:G:346:THR:HG22	1:G:348:GLU:H	1.43	0.83
1:H:57:LEU:C	1:H:101:MET:HE1	1.98	0.83
1:H:334:ARG:HA	1:H:355:MET:HE1	1.61	0.83
1:D:337:ARG:CB	1:D:355:MET:HE1	2.07	0.83
1:E:277:LEU:O	1:E:283:VAL:HG21	1.79	0.82
1:I:272:THR:CG2	1:I:273:PHE:HD1	1.90	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD23	1:A:125:MET:O	1.78	0.82
1:F:36:ASP:O	1:F:40:GLU:HG2	1.79	0.82
1:A:346:THR:HG22	1:A:348:GLU:H	1.43	0.82
1:C:275:GLU:CG	1:C:280:LYS:HZ3	1.92	0.82
1:A:125:MET:HE1	1:A:172:LEU:HD22	1.62	0.82
1:H:346:THR:HG22	1:H:348:GLU:H	1.42	0.82
1:I:271:SER:HB2	1:I:275:GLU:O	1.79	0.82
1:C:337:ARG:HB2	1:C:355:MET:HE3	1.62	0.82
1:G:96:GLN:O	1:G:101:MET:HG3	1.79	0.81
1:C:337:ARG:CB	1:C:355:MET:HE3	2.10	0.81
1:G:272:THR:HG22	1:G:273:PHE:CD1	2.15	0.81
1:F:275:GLU:HG3	1:F:280:LYS:NZ	1.96	0.81
1:A:253:MET:HE1	1:A:294:HIS:CA	2.03	0.81
1:I:337:ARG:CB	1:I:355:MET:HE3	2.11	0.81
1:D:35:ARG:HD2	3:D:3002:HOH:O	1.79	0.80
1:E:57:LEU:C	1:E:101:MET:HE1	2.02	0.80
1:G:382:LEU:HD13	1:H:279:LYS:HB2	1.61	0.80
1:C:272:THR:HG22	1:C:273:PHE:H	1.43	0.80
1:D:276:PRO:HD2	1:D:279:LYS:HB2	1.61	0.80
1:G:282:LEU:H	1:I:281:GLN:NE2	1.79	0.80
1:D:39:GLU:HG2	1:D:347:LEU:CD1	2.12	0.80
1:F:348:GLU:O	1:F:348:GLU:HG2	1.81	0.80
1:F:341:GLY:HA2	3:G:6007:HOH:O	1.81	0.80
1:C:314:THR:OG1	1:C:317:GLN:HG3	1.80	0.79
1:G:272:THR:HG22	1:G:273:PHE:H	1.44	0.79
1:A:337:ARG:CB	1:A:355:MET:HE1	2.13	0.79
1:D:349:TYR:O	1:D:350:HIS:HB2	1.80	0.79
1:F:339:ILE:O	2:G:6001:FAD:H4B	1.82	0.79
1:D:277:LEU:O	1:D:283:VAL:HG21	1.83	0.79
1:E:35:ARG:CG	1:E:35:ARG:HH11	1.95	0.79
1:G:7:LEU:HD13	1:G:10:LEU:HD12	1.64	0.79
1:C:275:GLU:CG	1:C:280:LYS:HZ1	1.91	0.78
1:F:299:LEU:HD13	1:I:299:LEU:HB3	1.65	0.78
1:I:346:THR:HG22	1:I:348:GLU:H	1.47	0.78
1:E:57:LEU:CB	1:E:101:MET:HE1	2.13	0.78
1:I:120:LEU:HD23	1:I:125:MET:O	1.83	0.78
1:F:207:LEU:H	1:F:357:ASN:HD22	1.31	0.78
1:G:275:GLU:HG3	1:G:280:LYS:NZ	1.99	0.78
1:C:120:LEU:CD2	1:C:125:MET:O	2.31	0.78
3:H:7042:HOH:O	1:I:203:ARG:HD2	1.82	0.77
1:F:15:GLU:O	1:F:18:VAL:HG22	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:272:THR:HG22	1:F:273:PHE:N	1.97	0.77
1:I:207:LEU:H	1:I:357:ASN:HD22	1.31	0.77
1:A:19:GLN:NE2	1:A:20:LYS:CE	2.40	0.77
1:F:58:GLY:HA3	1:F:101:MET:SD	2.24	0.77
1:H:348:GLU:CB	1:I:203:ARG:HH21	1.98	0.77
1:I:272:THR:O	1:I:274:GLY:N	2.17	0.77
1:A:100:VAL:C	1:A:103:PRO:HD2	2.06	0.77
1:C:271:SER:HB2	1:C:275:GLU:O	1.83	0.77
3:A:1038:HOH:O	1:D:346:THR:HG21	1.83	0.77
1:C:337:ARG:CZ	1:E:359:GLU:HG3	2.15	0.77
1:H:348:GLU:HB2	1:I:203:ARG:NH2	2.00	0.77
1:G:272:THR:CG2	1:G:273:PHE:CD1	2.68	0.76
1:G:38:TRP:HE1	1:G:357:ASN:HD21	1.31	0.76
1:H:120:LEU:HD23	1:H:125:MET:O	1.85	0.76
1:F:276:PRO:HG2	1:I:382:LEU:HD11	1.66	0.76
1:C:7:LEU:HD13	1:C:10:LEU:HD12	1.65	0.76
1:F:205:MET:HE2	1:G:205:MET:CE	2.16	0.76
1:A:100:VAL:O	1:A:103:PRO:HG2	1.85	0.76
1:D:50:ARG:O	1:D:54:LEU:CD1	2.33	0.76
1:A:359:GLU:HG3	1:D:337:ARG:CZ	2.15	0.76
1:D:207:LEU:H	1:D:357:ASN:HD22	1.33	0.76
1:F:346:THR:HG22	1:F:348:GLU:H	1.49	0.76
1:G:276:PRO:HD2	1:G:279:LYS:HB2	1.68	0.76
1:C:334:ARG:HA	1:C:355:MET:HE2	1.66	0.76
1:C:35:ARG:CD	1:E:203:ARG:CZ	2.63	0.76
1:H:200:GLU:OE1	1:H:202:LYS:NZ	2.19	0.76
1:H:348:GLU:CB	1:I:203:ARG:NH2	2.48	0.76
1:A:133:GLU:HG2	1:A:160:THR:O	1.86	0.75
1:H:346:THR:HG21	3:I:8048:HOH:O	1.85	0.75
1:A:337:ARG:CZ	1:D:359:GLU:HG3	2.16	0.75
1:F:149:ARG:HG2	1:F:156:VAL:HG12	1.68	0.75
1:A:334:ARG:HA	1:A:355:MET:CE	2.15	0.75
1:C:224:GLU:HG3	1:C:224:GLU:O	1.84	0.75
1:G:337:ARG:HB2	1:G:355:MET:HE3	1.68	0.75
1:D:136:GLY:HA2	2:D:3001:FAD:O2P	1.87	0.75
1:F:230:LYS:O	1:F:232:LEU:HD13	1.86	0.75
1:E:162:MET:HA	1:E:162:MET:HE3	1.68	0.75
1:F:320:LEU:HD23	1:I:4:PHE:HE2	1.51	0.75
1:G:202:LYS:HB2	1:G:203:ARG:HD2	1.67	0.75
1:A:346:THR:HG21	3:D:3043:HOH:O	1.87	0.75
1:H:74:ALA:O	1:H:78:ILE:HG23	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:125:MET:HE1	1:I:172:LEU:HD22	1.68	0.74
1:H:348:GLU:HA	1:I:203:ARG:NH2	2.01	0.74
1:D:120:LEU:HD23	1:D:125:MET:O	1.87	0.74
1:E:15:GLU:O	1:E:18:VAL:HG22	1.88	0.74
1:G:35:ARG:HG2	1:G:35:ARG:HH11	1.52	0.74
1:H:272:THR:CG2	1:H:273:PHE:CD1	2.71	0.74
1:I:156:VAL:HG11	3:I:8026:HOH:O	1.87	0.74
1:D:35:ARG:O	1:D:39:GLU:HG3	1.87	0.74
1:C:272:THR:CG2	1:E:139:ASP:HB2	2.13	0.74
1:I:57:LEU:HB3	1:I:101:MET:HE1	1.70	0.74
1:G:277:LEU:O	1:G:283:VAL:HG21	1.88	0.74
1:F:334:ARG:HA	1:F:355:MET:HE2	1.68	0.73
1:I:272:THR:CG2	1:I:273:PHE:H	1.85	0.73
1:C:232:LEU:O	1:C:235:LYS:HE3	1.88	0.73
1:F:277:LEU:O	1:F:283:VAL:HG21	1.88	0.73
1:A:272:THR:HG23	1:A:273:PHE:CD1	2.23	0.73
1:D:7:LEU:HD11	1:D:299:LEU:CD2	2.19	0.73
1:F:205:MET:CE	1:G:205:MET:CE	2.66	0.73
1:E:57:LEU:HB3	1:E:101:MET:CE	2.19	0.73
1:F:203:ARG:HG2	1:G:35:ARG:NH2	2.03	0.73
1:H:183:GLU:OE1	1:H:232:LEU:CD1	2.37	0.73
1:G:35:ARG:HG2	1:G:35:ARG:NH1	2.01	0.73
1:F:276:PRO:HG2	1:I:382:LEU:CD1	2.18	0.73
1:E:58:GLY:HA3	1:E:101:MET:SD	2.28	0.72
1:G:272:THR:C	1:G:274:GLY:N	2.41	0.72
1:F:281:GLN:HG2	1:I:373:LEU:HD11	1.69	0.72
1:A:299:LEU:HD13	1:C:299:LEU:HB3	1.70	0.72
1:I:35:ARG:HD2	3:I:8009:HOH:O	1.89	0.72
1:A:299:LEU:HB3	1:C:299:LEU:HD13	1.71	0.72
1:C:187:PHE:O	1:C:188:LEU:CG	2.34	0.72
1:E:272:THR:CG2	1:E:273:PHE:N	2.40	0.72
1:G:19:GLN:HE22	1:G:20:LYS:HE3	1.53	0.72
1:E:7:LEU:HD11	1:E:299:LEU:HD23	1.71	0.72
1:D:271:SER:OG	1:D:275:GLU:O	2.07	0.72
1:E:346:THR:HG22	1:E:348:GLU:H	1.53	0.72
1:A:337:ARG:NE	1:D:359:GLU:HG3	2.05	0.72
1:E:120:LEU:HD23	1:E:125:MET:O	1.90	0.72
1:A:207:LEU:H	1:A:357:ASN:HD22	1.38	0.71
1:D:275:GLU:HB2	1:D:276:PRO:HD3	1.73	0.71
1:F:35:ARG:NE	1:F:39:GLU:OE1	2.24	0.71
1:C:272:THR:CG2	1:C:273:PHE:CD1	2.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:334:ARG:HA	1:H:355:MET:CE	2.19	0.71
1:C:337:ARG:NE	1:E:359:GLU:HG3	2.06	0.71
1:G:272:THR:O	1:G:274:GLY:N	2.22	0.71
1:D:39:GLU:HG2	1:D:347:LEU:HD12	1.73	0.70
1:F:320:LEU:HD12	1:F:320:LEU:O	1.90	0.70
1:H:35:ARG:HD2	3:H:7042:HOH:O	1.90	0.70
1:I:133:GLU:HG2	1:I:160:THR:O	1.89	0.70
1:I:35:ARG:O	1:I:39:GLU:HG3	1.91	0.70
1:A:359:GLU:HG3	1:D:337:ARG:NE	2.06	0.70
1:G:57:LEU:CB	1:G:101:MET:HE1	2.21	0.70
1:G:253:MET:HE2	1:G:253:MET:HA	1.73	0.70
1:G:57:LEU:C	1:G:101:MET:HE1	2.10	0.70
1:H:272:THR:CG2	1:H:273:PHE:N	2.47	0.70
1:H:207:LEU:H	1:H:357:ASN:HD22	1.40	0.70
1:D:31:LEU:HG	1:D:31:LEU:O	1.91	0.70
1:G:19:GLN:HE22	1:G:20:LYS:CE	2.03	0.70
1:H:133:GLU:HG2	1:H:160:THR:O	1.91	0.70
1:A:359:GLU:HG3	1:D:337:ARG:NH2	2.07	0.70
1:F:203:ARG:CD	1:G:35:ARG:NH2	2.43	0.70
1:G:334:ARG:HA	1:G:355:MET:CE	2.21	0.70
1:C:197:GLN:HA	1:C:197:GLN:HE21	1.57	0.70
1:E:133:GLU:HG2	1:E:160:THR:O	1.92	0.70
1:A:190:PRO:O	1:A:193:THR:HG23	1.91	0.69
1:H:57:LEU:HG	1:H:96:GLN:HG2	1.73	0.69
1:E:162:MET:CE	1:E:163:TRP:H	2.03	0.69
1:C:39:GLU:OE1	1:E:203:ARG:HG2	1.93	0.69
1:E:334:ARG:HA	1:E:355:MET:CE	2.22	0.69
1:E:207:LEU:H	1:E:357:ASN:HD22	1.39	0.69
1:H:190:PRO:O	1:H:193:THR:HG23	1.92	0.69
1:A:100:VAL:O	1:A:103:PRO:HD2	1.92	0.69
1:C:58:GLY:CA	1:C:101:MET:SD	2.80	0.69
1:E:35:ARG:HB2	1:E:35:ARG:NH1	2.08	0.69
1:G:19:GLN:NE2	1:G:20:LYS:CE	2.54	0.69
1:H:272:THR:CG2	1:H:273:PHE:HD1	2.05	0.69
1:H:337:ARG:CB	1:H:355:MET:HE3	2.22	0.69
1:H:359:GLU:HG3	1:I:337:ARG:NE	2.08	0.69
1:A:135:ASP:OD1	1:A:145:LYS:HE3	1.93	0.69
1:C:327:TRP:O	1:C:331:GLN:HG3	1.93	0.69
1:D:157:LEU:HD13	1:D:222:VAL:HG23	1.73	0.69
1:C:125:MET:HE1	1:C:172:LEU:HD22	1.74	0.69
1:F:203:ARG:HD2	3:F:5031:HOH:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:LEU:HB3	1:G:101:MET:CE	2.22	0.69
1:H:272:THR:HG22	1:H:273:PHE:HD1	1.58	0.69
1:C:253:MET:CE	1:C:294:HIS:CA	2.54	0.68
1:D:57:LEU:C	1:D:101:MET:HE1	2.13	0.68
1:G:190:PRO:O	1:G:193:THR:HG23	1.92	0.68
1:F:205:MET:CE	1:G:205:MET:HE1	2.23	0.68
1:D:7:LEU:HD11	1:D:299:LEU:HD23	1.76	0.68
1:H:348:GLU:CA	1:I:203:ARG:NH2	2.56	0.68
1:G:197:GLN:HE21	1:G:197:GLN:HA	1.59	0.68
1:G:337:ARG:HG3	1:G:355:MET:HE1	1.75	0.68
1:D:334:ARG:HA	1:D:355:MET:CE	2.23	0.68
1:H:359:GLU:HG3	1:I:337:ARG:CZ	2.23	0.68
1:I:57:LEU:HG	1:I:96:GLN:HG2	1.75	0.68
1:F:299:LEU:HB3	1:I:299:LEU:HD13	1.74	0.68
1:E:57:LEU:HG	1:E:96:GLN:HG2	1.75	0.68
1:H:35:ARG:O	1:H:39:GLU:HG2	1.94	0.68
1:C:337:ARG:HB2	1:C:355:MET:CE	2.23	0.68
1:G:282:LEU:HG	1:I:281:GLN:HB3	1.75	0.68
1:H:109:SER:OG	1:H:112:GLN:HG3	1.93	0.68
1:A:197:GLN:HE21	1:A:197:GLN:HA	1.59	0.68
1:D:156:VAL:HG21	1:D:219:GLU:OE2	1.94	0.68
1:H:57:LEU:HB3	1:H:101:MET:HE1	1.76	0.68
1:D:276:PRO:HD2	1:D:279:LYS:CB	2.24	0.67
1:F:126:VAL:HG13	1:F:169:LEU:O	1.93	0.67
1:H:35:ARG:CD	3:H:7042:HOH:O	2.42	0.67
1:H:346:THR:HG23	1:I:203:ARG:HB2	1.75	0.67
1:D:272:THR:HG22	1:D:273:PHE:H	1.58	0.67
1:G:207:LEU:H	1:G:357:ASN:HD22	1.42	0.67
1:G:78:ILE:HG13	1:G:79:CYS:N	2.09	0.67
1:C:337:ARG:CB	1:C:355:MET:CE	2.72	0.67
1:I:272:THR:CG2	1:I:273:PHE:N	2.46	0.67
1:H:253:MET:HE3	1:H:294:HIS:HA	1.73	0.67
1:H:203:ARG:HH21	1:I:39:GLU:HG2	1.59	0.67
1:C:223:PRO:HG2	1:C:226:LEU:HB2	1.76	0.67
1:E:190:PRO:O	1:E:193:THR:HG23	1.93	0.67
1:D:50:ARG:O	1:D:54:LEU:HD12	1.94	0.67
1:F:275:GLU:HG3	1:F:280:LYS:HZ2	1.57	0.67
1:F:284:GLN:NE2	1:I:376:GLY:HA3	2.10	0.67
1:C:207:LEU:H	1:C:357:ASN:HD22	1.43	0.66
1:G:78:ILE:HD11	1:G:93:VAL:HG11	1.77	0.66
1:A:102:TYR:N	1:A:103:PRO:HD2	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:ARG:CG	1:G:35:ARG:HH21	2.08	0.66
1:D:337:ARG:HG3	1:D:355:MET:HE1	1.76	0.66
1:E:7:LEU:HD13	1:E:10:LEU:HD12	1.75	0.66
1:I:190:PRO:HB2	1:I:193:THR:HG22	1.78	0.66
1:D:50:ARG:O	1:D:54:LEU:HD13	1.94	0.66
1:C:35:ARG:CD	1:E:203:ARG:NH1	2.56	0.66
1:D:38:TRP:HE1	1:D:357:ASN:HD21	1.42	0.66
1:F:172:LEU:HD11	1:F:188:LEU:HB3	1.76	0.66
3:H:7048:HOH:O	1:I:341:GLY:HA2	1.94	0.66
1:F:133:GLU:HG2	1:F:160:THR:O	1.94	0.66
1:I:15:GLU:O	1:I:18:VAL:HG22	1.97	0.66
1:D:262:GLU:OE1	1:D:349:TYR:O	2.14	0.65
1:F:223:PRO:HG2	1:F:226:LEU:HB2	1.77	0.65
1:C:203:ARG:HB2	1:E:346:THR:HG23	1.78	0.65
1:D:190:PRO:O	1:D:193:THR:HG23	1.97	0.65
1:F:207:LEU:H	1:F:357:ASN:ND2	1.94	0.65
1:F:253:MET:HE2	1:F:294:HIS:HA	1.71	0.65
1:I:190:PRO:O	1:I:193:THR:HG23	1.95	0.65
1:D:349:TYR:O	1:D:350:HIS:CB	2.44	0.65
1:E:223:PRO:HG2	1:E:226:LEU:HB2	1.79	0.65
3:H:7037:HOH:O	1:I:346:THR:HG21	1.96	0.65
1:I:57:LEU:CA	1:I:101:MET:HE1	2.25	0.65
1:C:334:ARG:HA	1:C:355:MET:CE	2.25	0.65
1:F:14:GLU:O	1:F:18:VAL:HG13	1.97	0.65
1:F:203:ARG:CG	1:G:35:ARG:NH2	2.60	0.65
1:H:223:PRO:HG2	1:H:226:LEU:HB2	1.78	0.65
1:C:314:THR:HG1	1:C:317:GLN:HG3	1.61	0.65
1:F:57:LEU:HG	1:F:96:GLN:HG2	1.78	0.65
1:G:15:GLU:O	1:G:18:VAL:HG22	1.97	0.65
1:I:337:ARG:HG3	1:I:355:MET:HE3	1.77	0.65
1:C:304:LEU:HD21	1:C:318:VAL:HA	1.79	0.65
1:D:35:ARG:CD	3:D:3002:HOH:O	2.42	0.65
1:F:109:SER:OG	1:F:112:GLN:HG3	1.97	0.65
1:A:101:MET:HE1	1:A:121:ALA:CA	2.24	0.65
1:C:78:ILE:HG13	1:C:79:CYS:N	2.12	0.65
1:C:7:LEU:CD1	1:C:10:LEU:HD12	2.27	0.65
1:G:270:ARG:HB3	1:G:277:LEU:HD22	1.77	0.65
1:F:190:PRO:O	1:F:193:THR:HG23	1.97	0.64
1:H:35:ARG:HG3	1:H:35:ARG:HH11	1.63	0.64
1:A:337:ARG:HB2	1:A:355:MET:CE	2.27	0.64
1:C:116:PHE:CD1	1:C:125:MET:HE1	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:280:LYS:HB2	1:H:283:VAL:HG13	1.79	0.64
1:I:78:ILE:HG13	1:I:79:CYS:N	2.12	0.64
1:D:337:ARG:HB2	1:D:355:MET:CE	2.28	0.64
1:F:38:TRP:HE1	1:F:357:ASN:HD21	1.44	0.64
1:E:7:LEU:HD11	1:E:299:LEU:CD2	2.26	0.64
3:D:3042:HOH:O	1:E:312:LYS:HD2	1.96	0.64
1:E:78:ILE:HG13	1:E:79:CYS:N	2.10	0.64
1:C:272:THR:C	1:C:274:GLY:H	2.01	0.64
1:C:57:LEU:HG	1:C:96:GLN:HG2	1.79	0.64
1:H:203:ARG:HH21	1:I:39:GLU:CG	2.10	0.64
1:I:207:LEU:H	1:I:357:ASN:ND2	1.95	0.64
1:D:57:LEU:HG	1:D:96:GLN:HG2	1.78	0.64
1:G:275:GLU:HG3	1:G:280:LYS:HZ2	1.63	0.64
1:H:270:ARG:HB3	1:H:277:LEU:HD22	1.78	0.64
1:D:337:ARG:CG	1:D:355:MET:HE1	2.26	0.64
1:E:334:ARG:HA	1:E:355:MET:HE2	1.80	0.64
1:E:35:ARG:CB	1:E:35:ARG:HH11	2.10	0.64
1:C:324:GLN:O	1:C:328:LYS:HD2	1.98	0.64
1:D:270:ARG:HB3	1:D:277:LEU:HD22	1.79	0.64
1:E:232:LEU:O	1:E:235:LYS:HE3	1.98	0.64
1:D:337:ARG:CB	1:D:355:MET:CE	2.75	0.64
1:I:271:SER:CB	1:I:275:GLU:O	2.46	0.64
3:G:6038:HOH:O	1:H:312:LYS:HD3	1.97	0.64
1:A:190:PRO:HB2	1:A:193:THR:HG22	1.78	0.63
1:A:282:LEU:H	1:E:281:GLN:NE2	1.97	0.63
1:E:207:LEU:H	1:E:357:ASN:ND2	1.97	0.63
1:G:260:TYR:OH	1:H:379:ILE:HG23	1.98	0.63
1:I:57:LEU:CB	1:I:101:MET:HE1	2.28	0.63
1:C:80:TYR:CE1	1:C:253:MET:O	2.51	0.63
1:H:19:GLN:NE2	1:H:20:LYS:HE3	2.13	0.63
1:E:144:MET:SD	1:E:178:LYS:HG3	2.39	0.63
1:G:74:ALA:O	1:G:78:ILE:HG23	1.98	0.63
1:F:320:LEU:HD23	1:I:4:PHE:CD2	2.33	0.63
1:A:281:GLN:HB2	1:E:281:GLN:HB2	1.79	0.63
1:I:7:LEU:HD11	1:I:299:LEU:HD23	1.80	0.63
1:C:35:ARG:HH11	1:C:35:ARG:HG3	1.63	0.63
1:E:337:ARG:CB	1:E:355:MET:HE3	2.29	0.63
1:G:35:ARG:CG	1:G:35:ARG:HH11	2.12	0.63
1:C:7:LEU:HD11	1:C:299:LEU:HD23	1.81	0.62
1:H:7:LEU:HD13	1:H:10:LEU:HD12	1.80	0.62
1:I:337:ARG:HB2	1:I:355:MET:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:PRO:HB2	1:D:193:THR:HG22	1.81	0.62
1:D:197:GLN:HE21	1:D:197:GLN:HA	1.64	0.62
1:D:207:LEU:H	1:D:357:ASN:ND2	1.96	0.62
1:F:7:LEU:HD11	1:F:299:LEU:HD23	1.80	0.62
1:A:337:ARG:NH2	1:D:359:GLU:HG3	2.14	0.62
1:I:74:ALA:O	1:I:78:ILE:HG23	1.98	0.62
1:A:253:MET:CE	1:A:294:HIS:CA	2.64	0.62
1:C:19:GLN:NE2	1:C:20:LYS:HE3	2.14	0.62
1:D:25:PHE:CD2	1:D:54:LEU:HD22	2.35	0.62
1:G:190:PRO:HB2	1:G:193:THR:HG22	1.81	0.62
1:D:334:ARG:HA	1:D:355:MET:HE2	1.80	0.62
1:I:337:ARG:HB2	1:I:355:MET:CE	2.29	0.62
1:A:100:VAL:O	1:A:103:PRO:CG	2.46	0.62
1:C:282:LEU:H	1:D:281:GLN:NE2	1.97	0.62
1:G:125:MET:HE1	1:G:172:LEU:HD22	1.82	0.62
1:C:272:THR:O	1:C:274:GLY:N	2.29	0.62
1:C:310:GLU:OE1	1:C:312:LYS:HE2	1.99	0.62
1:H:205:MET:CE	1:I:205:MET:CE	2.78	0.62
1:C:156:VAL:HG11	3:C:2051:HOH:O	2.00	0.62
1:C:277:LEU:O	1:C:283:VAL:CG2	2.44	0.62
1:F:139:ASP:HB2	1:G:272:THR:CG2	2.20	0.62
1:A:337:ARG:CB	1:A:355:MET:CE	2.77	0.61
1:C:242:THR:CG2	1:C:318:VAL:HG21	2.30	0.61
1:C:7:LEU:HD13	1:C:10:LEU:CD1	2.30	0.61
1:F:346:THR:CG2	3:G:6039:HOH:O	2.48	0.61
1:I:7:LEU:HD13	1:I:10:LEU:HD12	1.83	0.61
1:H:349:TYR:O	1:H:350:HIS:HB2	2.00	0.61
1:C:262:GLU:OE2	1:C:349:TYR:O	2.18	0.61
1:D:346:THR:HG22	1:D:348:GLU:N	2.14	0.61
1:I:337:ARG:CG	1:I:355:MET:HE3	2.30	0.61
1:F:314:THR:OG1	1:F:317:GLN:HG3	2.00	0.61
1:F:8:GLU:HA	1:F:11:LEU:HD12	1.82	0.61
1:I:36:ASP:O	1:I:40:GLU:HG2	2.00	0.61
1:E:149:ARG:O	1:E:155:TRP:HA	2.00	0.61
1:H:346:THR:HA	1:I:203:ARG:O	2.00	0.61
1:H:253:MET:CE	1:H:294:HIS:CA	2.67	0.61
1:A:253:MET:HE3	1:A:256:LEU:HD13	1.81	0.61
1:D:337:ARG:HB2	1:D:355:MET:HE1	1.80	0.61
1:F:200:GLU:OE1	1:F:202:LYS:NZ	2.34	0.61
1:G:337:ARG:CB	1:G:355:MET:CE	2.79	0.61
1:H:346:THR:HG22	1:H:348:GLU:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:15:GLU:O	1:H:18:VAL:HG22	2.01	0.61
1:H:38:TRP:HE1	1:H:357:ASN:HD21	1.48	0.61
1:I:223:PRO:HG2	1:I:226:LEU:HB2	1.82	0.61
1:E:35:ARG:NH1	1:E:35:ARG:HG3	2.14	0.61
1:F:276:PRO:HD2	1:F:279:LYS:HB2	1.83	0.61
1:F:78:ILE:HG13	1:F:79:CYS:N	2.16	0.61
1:G:133:GLU:HG2	1:G:160:THR:O	2.00	0.61
1:H:272:THR:HG22	1:H:273:PHE:CD1	2.35	0.61
1:C:286:LYS:O	1:C:290:MET:HG3	2.00	0.60
1:I:334:ARG:HA	1:I:355:MET:CE	2.31	0.60
1:F:190:PRO:HB2	1:F:193:THR:HG22	1.83	0.60
1:C:38:TRP:HE1	1:C:357:ASN:HD21	1.49	0.60
1:D:253:MET:HE1	1:D:294:HIS:CA	2.18	0.60
1:D:234:LEU:HD22	1:D:238:LEU:HG	1.82	0.60
1:D:31:LEU:HD12	1:D:85:VAL:HG13	1.83	0.60
1:H:57:LEU:CA	1:H:101:MET:HE1	2.31	0.60
1:H:262:GLU:OE1	1:H:349:TYR:O	2.19	0.60
1:C:190:PRO:O	1:C:193:THR:HG23	2.02	0.60
1:G:200:GLU:OE1	1:G:202:LYS:NZ	2.34	0.60
1:I:140:PRO:HG2	1:I:141:TYR:N	2.16	0.60
1:I:57:LEU:HB3	1:I:101:MET:CE	2.31	0.60
1:C:361:VAL:HG13	1:C:364:TYR:CE1	2.36	0.60
1:D:15:GLU:O	1:D:18:VAL:HG22	2.01	0.60
1:I:337:ARG:CB	1:I:355:MET:CE	2.80	0.60
1:D:162:MET:CE	1:D:162:MET:HA	2.31	0.60
1:G:120:LEU:HD23	1:G:125:MET:O	2.01	0.60
1:I:78:ILE:HD11	1:I:93:VAL:HG11	1.83	0.60
1:C:359:GLU:HG3	1:E:337:ARG:NE	2.17	0.60
1:C:36:ASP:O	1:C:40:GLU:HG2	2.02	0.60
1:F:35:ARG:NH2	1:F:39:GLU:OE1	2.34	0.60
1:G:223:PRO:HG2	1:G:226:LEU:HB2	1.84	0.60
1:F:320:LEU:HD12	1:F:320:LEU:C	2.22	0.59
1:H:337:ARG:NH2	1:I:359:GLU:HG3	2.17	0.59
1:F:172:LEU:HD11	1:F:188:LEU:C	2.22	0.59
1:F:334:ARG:HA	1:F:355:MET:CE	2.32	0.59
1:G:126:VAL:O	1:G:170:ALA:HA	2.01	0.59
1:G:203:ARG:HD3	3:G:6039:HOH:O	2.02	0.59
1:G:299:LEU:HD12	1:H:300:LEU:HD23	1.83	0.59
1:C:346:THR:HG22	1:C:348:GLU:N	2.17	0.59
1:D:223:PRO:HG2	1:D:226:LEU:HB2	1.83	0.59
1:I:197:GLN:HA	1:I:197:GLN:HE21	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:THR:HG21	1:E:273:PHE:CD1	2.36	0.59
1:E:337:ARG:HB2	1:E:355:MET:HE3	1.84	0.59
1:H:253:MET:HE1	1:H:294:HIS:CA	2.21	0.59
1:A:200:GLU:OE1	1:A:202:LYS:NZ	2.36	0.59
1:D:16:LYS:O	1:D:20:LYS:HG2	2.02	0.59
1:F:275:GLU:HG3	1:F:280:LYS:HZ1	1.68	0.59
1:A:207:LEU:H	1:A:357:ASN:ND2	1.99	0.59
1:D:144:MET:SD	1:D:178:LYS:HG3	2.43	0.59
1:F:197:GLN:HA	1:F:197:GLN:HE21	1.67	0.59
1:G:272:THR:CG2	1:G:273:PHE:N	2.50	0.59
1:I:109:SER:OG	1:I:112:GLN:HG3	2.02	0.59
1:C:275:GLU:CD	1:C:280:LYS:HZ3	2.05	0.59
1:C:346:THR:HG21	3:E:4040:HOH:O	2.01	0.59
1:E:57:LEU:C	1:E:101:MET:CE	2.71	0.59
1:H:78:ILE:HG13	1:H:79:CYS:N	2.17	0.59
1:H:337:ARG:CZ	1:I:359:GLU:HG3	2.32	0.59
1:A:277:LEU:HD11	2:D:3001:FAD:O4B	2.03	0.59
1:C:272:THR:CG2	1:C:273:PHE:N	2.53	0.59
1:C:78:ILE:HD11	1:C:93:VAL:HG11	1.83	0.59
1:E:190:PRO:HB2	1:E:193:THR:HG22	1.84	0.59
1:E:23:ARG:O	1:E:27:GLU:HB2	2.02	0.59
1:E:7:LEU:CD1	1:E:10:LEU:HD12	2.33	0.59
1:A:346:THR:HG22	1:A:348:GLU:N	2.16	0.59
1:H:304:LEU:HD21	1:H:318:VAL:HA	1.85	0.59
1:I:7:LEU:HD11	1:I:299:LEU:CD2	2.32	0.59
1:I:38:TRP:HE1	1:I:357:ASN:HD21	1.51	0.59
1:I:234:LEU:HD22	1:I:238:LEU:HG	1.84	0.58
1:F:205:MET:HE2	1:G:205:MET:HE1	1.83	0.58
1:G:282:LEU:H	1:I:281:GLN:HE21	1.50	0.58
1:E:7:LEU:HD13	1:E:10:LEU:CD1	2.33	0.58
1:H:190:PRO:HB2	1:H:193:THR:HG22	1.85	0.58
1:C:35:ARG:HD2	1:E:203:ARG:HH12	1.66	0.58
1:F:74:ALA:O	1:F:78:ILE:HG23	2.03	0.58
1:I:19:GLN:NE2	1:I:20:LYS:HE3	2.18	0.58
1:C:190:PRO:HB2	1:C:193:THR:HG22	1.84	0.58
1:F:272:THR:CG2	1:F:273:PHE:N	2.66	0.58
1:G:231:ALA:O	1:G:232:LEU:HD12	2.03	0.58
1:E:304:LEU:HD21	1:E:318:VAL:HA	1.85	0.58
1:G:272:THR:HG21	1:G:273:PHE:CD1	2.38	0.58
1:G:304:LEU:HD21	1:G:318:VAL:HA	1.85	0.58
1:I:271:SER:HA	1:I:276:PRO:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:PRO:HG2	1:A:226:LEU:HB2	1.83	0.58
1:A:78:ILE:HG13	1:A:79:CYS:N	2.18	0.58
1:C:360:THR:HG21	2:C:2001:FAD:HM73	1.85	0.58
1:G:253:MET:CE	1:G:253:MET:HA	2.33	0.58
1:C:96:GLN:HG3	1:C:101:MET:HE2	1.85	0.58
1:D:231:ALA:O	1:D:232:LEU:HD12	2.04	0.57
1:D:74:ALA:O	1:D:78:ILE:HG23	2.03	0.57
1:E:74:ALA:O	1:E:78:ILE:HG23	2.04	0.57
1:H:203:ARG:NH2	1:I:39:GLU:HB3	2.19	0.57
1:C:337:ARG:NH2	1:E:359:GLU:HG3	2.19	0.57
1:C:74:ALA:O	1:C:78:ILE:HG23	2.04	0.57
1:D:36:ASP:O	1:D:40:GLU:CG	2.43	0.57
1:G:278:ALA:HB3	1:H:382:LEU:HD12	1.86	0.57
1:I:110:GLU:OE2	1:I:114:ARG:NH2	2.37	0.57
1:I:349:TYR:O	1:I:350:HIS:HB2	2.03	0.57
1:C:361:VAL:HG13	1:C:364:TYR:HE1	1.68	0.57
1:E:12:THR:OG1	1:E:15:GLU:HG3	2.04	0.57
1:E:234:LEU:HD22	1:E:238:LEU:HG	1.86	0.57
1:E:272:THR:CG2	1:E:273:PHE:H	2.00	0.57
1:F:207:LEU:HD22	1:F:360:THR:HG21	1.85	0.57
1:I:16:LYS:O	1:I:20:LYS:HG2	2.04	0.57
1:I:346:THR:HG22	1:I:348:GLU:N	2.18	0.57
1:C:107:TYR:HA	1:C:230:LYS:HE3	1.86	0.57
1:C:281:GLN:HB2	1:D:281:GLN:HB2	1.86	0.57
1:E:57:LEU:CA	1:E:101:MET:HE1	2.34	0.57
1:A:12:THR:OG1	1:A:15:GLU:HG3	2.05	0.57
1:D:7:LEU:HD11	1:D:299:LEU:HD21	1.87	0.57
1:D:58:GLY:N	1:D:101:MET:HE1	2.19	0.57
1:A:109:SER:OG	1:A:112:GLN:HG3	2.05	0.57
1:A:337:ARG:HG3	1:A:355:MET:HE1	1.86	0.57
1:C:339:ILE:O	2:E:4001:FAD:H4B	2.03	0.57
1:G:65:TYR:OH	1:G:110:GLU:OE2	2.14	0.57
1:E:82:LEU:HD11	1:E:93:VAL:HG21	1.85	0.57
1:F:205:MET:HE1	1:G:205:MET:HE1	1.87	0.57
1:D:379:ILE:HG12	1:E:291:LEU:HD22	1.87	0.57
1:F:110:GLU:OE2	1:F:114:ARG:NH2	2.38	0.57
1:G:19:GLN:HE22	1:G:20:LYS:NZ	2.02	0.57
1:A:260:TYR:HA	1:A:290:MET:HE1	1.86	0.57
1:D:200:GLU:OE1	1:D:202:LYS:NZ	2.37	0.57
1:F:107:TYR:HA	1:F:230:LYS:HB2	1.87	0.57
1:H:253:MET:HE3	1:H:256:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:VAL:HG21	1:C:219:GLU:OE2	2.05	0.57
1:H:7:LEU:HD11	1:H:299:LEU:HD23	1.87	0.57
1:A:383:ASN:O	1:C:279:LYS:HE3	2.04	0.56
1:E:272:THR:C	1:E:274:GLY:H	2.08	0.56
1:C:111:GLU:O	1:C:115:GLU:HB2	2.05	0.56
1:C:359:GLU:HG3	1:E:337:ARG:CZ	2.35	0.56
1:E:110:GLU:OE2	1:E:114:ARG:NH2	2.38	0.56
1:A:74:ALA:O	1:A:78:ILE:HG23	2.04	0.56
1:F:156:VAL:HG21	1:F:219:GLU:OE2	2.05	0.56
1:G:202:LYS:CB	1:G:203:ARG:HD2	2.36	0.56
1:H:337:ARG:NE	1:I:359:GLU:HG3	2.20	0.56
1:C:7:LEU:HD11	1:C:299:LEU:CD2	2.35	0.56
1:E:272:THR:HG22	1:E:273:PHE:HD1	1.65	0.56
1:E:38:TRP:HE1	1:E:357:ASN:HD21	1.52	0.56
1:C:260:TYR:O	1:C:264:VAL:HG13	2.05	0.56
1:F:231:ALA:O	1:F:232:LEU:HD12	2.05	0.56
1:D:109:SER:OG	1:D:112:GLN:HG3	2.06	0.56
1:D:48:ILE:HB	1:D:49:PRO:CD	2.36	0.56
1:D:78:ILE:HD11	1:D:93:VAL:HG11	1.87	0.56
1:F:337:ARG:CB	1:F:355:MET:HE1	2.36	0.56
1:A:203:ARG:HB2	1:D:346:THR:HG23	1.87	0.56
1:D:35:ARG:HG3	1:D:35:ARG:HH11	1.69	0.56
1:G:346:THR:HG22	1:G:348:GLU:N	2.17	0.56
1:C:337:ARG:CG	1:C:355:MET:HE3	2.35	0.56
1:D:260:TYR:HA	1:D:290:MET:HE1	1.88	0.56
1:D:272:THR:CG2	1:D:273:PHE:HD1	2.05	0.56
1:F:310:GLU:OE1	1:F:312:LYS:CE	2.54	0.56
1:H:337:ARG:HB2	1:H:355:MET:CE	2.36	0.56
1:I:334:ARG:HA	1:I:355:MET:HE1	1.87	0.56
1:A:100:VAL:O	1:A:103:PRO:CD	2.53	0.56
1:C:110:GLU:OE2	1:C:114:ARG:NH2	2.38	0.56
1:C:275:GLU:HG3	1:C:280:LYS:NZ	2.17	0.56
1:F:126:VAL:CG1	1:F:169:LEU:O	2.53	0.56
1:F:16:LYS:O	1:F:20:LYS:HG2	2.06	0.56
1:H:16:LYS:O	1:H:20:LYS:HG2	2.06	0.56
1:H:207:LEU:H	1:H:357:ASN:ND2	2.01	0.56
1:G:379:ILE:CD1	1:H:288:ALA:HA	2.35	0.56
1:G:12:THR:OG1	1:G:15:GLU:HG3	2.06	0.55
1:H:149:ARG:NH2	1:H:219:GLU:OE2	2.39	0.55
1:D:260:TYR:O	1:D:264:VAL:HG13	2.05	0.55
1:E:310:GLU:HG3	1:E:312:LYS:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:291:LEU:HD22	1:H:379:ILE:HG12	1.88	0.55
1:G:310:GLU:HG3	1:G:312:LYS:HE2	1.88	0.55
1:C:163:TRP:CZ3	1:C:201:VAL:HG11	2.41	0.55
1:F:80:TYR:HE1	1:F:253:MET:HB3	1.72	0.55
3:F:5031:HOH:O	1:G:346:THR:CG2	2.53	0.55
1:H:149:ARG:HG3	1:H:156:VAL:HG12	1.89	0.55
1:I:207:LEU:HD22	1:I:360:THR:HG21	1.87	0.55
1:A:275:GLU:HG3	1:A:280:LYS:HZ2	1.72	0.55
1:D:78:ILE:HG13	1:D:79:CYS:N	2.20	0.55
1:I:304:LEU:HD21	1:I:318:VAL:HA	1.87	0.55
1:A:39:GLU:OE2	1:D:203:ARG:HD2	2.05	0.55
1:F:172:LEU:HD11	1:F:188:LEU:CB	2.37	0.55
1:F:272:THR:CG2	1:F:273:PHE:HD1	2.20	0.55
1:F:7:LEU:HD11	1:F:299:LEU:CD2	2.36	0.55
1:F:337:ARG:HG3	1:F:355:MET:HE1	1.89	0.55
1:G:7:LEU:HD11	1:G:299:LEU:HD23	1.89	0.55
1:F:12:THR:OG1	1:F:15:GLU:HG3	2.07	0.55
1:G:275:GLU:HB3	1:G:279:LYS:HD3	1.88	0.55
1:A:57:LEU:HG	1:A:96:GLN:HG2	1.89	0.55
1:F:346:THR:HG21	3:G:6039:HOH:O	2.06	0.55
1:F:35:ARG:HH21	1:F:39:GLU:CD	2.10	0.55
1:G:207:LEU:H	1:G:357:ASN:ND2	2.05	0.55
1:H:23:ARG:O	1:H:27:GLU:HB2	2.07	0.55
1:A:282:LEU:HG	1:E:281:GLN:HE21	1.72	0.55
1:E:31:LEU:HB3	1:E:32:PRO:CD	2.37	0.55
1:H:57:LEU:HB3	1:H:101:MET:CE	2.36	0.55
1:E:337:ARG:HB2	1:E:355:MET:CE	2.37	0.54
1:G:155:TRP:CD1	1:G:155:TRP:N	2.75	0.54
1:G:163:TRP:HZ3	1:G:201:VAL:HG11	1.72	0.54
1:G:35:ARG:HH22	1:G:39:GLU:CD	2.10	0.54
1:C:163:TRP:HZ3	1:C:201:VAL:HG11	1.72	0.54
1:A:359:GLU:CG	1:D:337:ARG:NE	2.71	0.54
1:E:15:GLU:OE2	1:E:73:ALA:HB3	2.07	0.54
1:G:262:GLU:OE1	1:G:349:TYR:O	2.25	0.54
1:G:276:PRO:HD2	1:G:279:LYS:CB	2.36	0.54
1:H:149:ARG:HG2	1:H:156:VAL:CG1	2.37	0.54
1:H:203:ARG:NH2	1:I:39:GLU:CG	2.71	0.54
1:H:149:ARG:CG	1:H:156:VAL:HG12	2.38	0.54
1:D:38:TRP:HE1	1:D:357:ASN:ND2	2.05	0.54
1:F:304:LEU:HD21	1:F:318:VAL:HA	1.90	0.54
1:H:163:TRP:CZ3	1:H:201:VAL:HG11	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:ARG:HH11	1:I:35:ARG:HG3	1.72	0.54
1:C:310:GLU:HG3	1:C:312:LYS:HE2	1.88	0.54
1:E:272:THR:HG21	1:E:273:PHE:CE1	2.43	0.54
1:G:163:TRP:CZ3	1:G:201:VAL:HG11	2.42	0.54
1:H:337:ARG:CB	1:H:355:MET:CE	2.86	0.54
1:I:144:MET:SD	1:I:178:LYS:HG3	2.48	0.54
1:C:16:LYS:O	1:C:20:LYS:HG2	2.07	0.54
1:A:337:ARG:NE	1:D:359:GLU:CG	2.71	0.54
1:H:57:LEU:CB	1:H:101:MET:HE1	2.37	0.54
1:F:78:ILE:HD11	1:F:93:VAL:HG11	1.89	0.54
1:I:200:GLU:OE1	1:I:202:LYS:NZ	2.40	0.54
1:C:203:ARG:HB2	3:C:2033:HOH:O	2.08	0.54
1:E:253:MET:CE	1:E:294:HIS:CA	2.73	0.54
1:F:253:MET:HE3	1:F:256:LEU:HD13	1.89	0.54
1:F:289:GLU:HB2	3:I:8065:HOH:O	2.07	0.54
2:H:7001:FAD:H4B	1:I:339:ILE:O	2.08	0.54
1:A:337:ARG:CG	1:A:355:MET:HE1	2.37	0.54
1:H:256:LEU:HD23	1:H:256:LEU:O	2.08	0.54
1:D:304:LEU:HD21	1:D:318:VAL:HA	1.90	0.54
1:E:109:SER:OG	1:E:112:GLN:HG3	2.08	0.54
1:E:19:GLN:NE2	1:E:20:LYS:HE3	2.23	0.54
1:G:57:LEU:C	1:G:101:MET:CE	2.77	0.54
1:E:272:THR:CG2	1:E:273:PHE:HD1	2.18	0.53
1:F:280:LYS:O	1:F:283:VAL:HG22	2.08	0.53
1:H:58:GLY:N	1:H:101:MET:HE1	2.23	0.53
1:H:7:LEU:CD1	1:H:10:LEU:HD12	2.38	0.53
1:A:231:ALA:O	1:A:232:LEU:HD12	2.08	0.53
1:A:260:TYR:HB2	1:A:290:MET:HE2	1.90	0.53
1:A:272:THR:CG2	1:A:273:PHE:CD1	2.92	0.53
1:A:304:LEU:HD21	1:A:318:VAL:HA	1.90	0.53
1:C:234:LEU:HD13	1:C:238:LEU:HD11	1.90	0.53
1:C:272:THR:C	1:C:274:GLY:N	2.62	0.53
1:E:272:THR:CG2	1:E:273:PHE:CE1	2.90	0.53
1:E:310:GLU:OE1	1:E:312:LYS:HE3	2.08	0.53
1:E:35:ARG:HB2	1:E:35:ARG:HH11	1.68	0.53
1:G:281:GLN:HB2	1:I:281:GLN:HB2	1.90	0.53
1:G:337:ARG:CB	1:G:355:MET:HE3	2.35	0.53
1:H:58:GLY:HA3	1:H:101:MET:SD	2.48	0.53
1:I:253:MET:HE1	1:I:294:HIS:CA	2.07	0.53
1:I:39:GLU:HG2	1:I:347:LEU:HD12	1.90	0.53
1:C:271:SER:CB	1:C:276:PRO:HA	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:ARG:HG3	1:C:355:MET:HE3	1.90	0.53
1:F:262:GLU:OE1	1:F:349:TYR:O	2.27	0.53
1:A:38:TRP:HE1	1:A:357:ASN:HD21	1.55	0.53
1:C:337:ARG:NE	1:E:359:GLU:CG	2.71	0.53
1:C:78:ILE:HD12	1:C:82:LEU:CD1	2.38	0.53
1:E:48:ILE:HG22	3:E:4060:HOH:O	2.08	0.53
1:F:19:GLN:NE2	1:F:20:LYS:HE3	2.23	0.53
1:A:206:SER:HB3	1:D:345:ILE:HB	1.89	0.53
1:E:327:TRP:CE3	1:E:362:TYR:CE1	2.95	0.53
1:G:314:THR:OG1	1:G:317:GLN:HG3	2.09	0.53
1:F:292:ALA:CB	1:I:320:LEU:HD11	2.38	0.53
1:H:359:GLU:HG3	1:I:337:ARG:NH2	2.24	0.53
1:C:270:ARG:NH2	3:C:2048:HOH:O	2.41	0.53
1:E:78:ILE:HD11	1:E:93:VAL:HG11	1.90	0.53
1:H:310:GLU:OE1	3:H:7004:HOH:O	2.18	0.53
1:F:82:LEU:HD11	1:F:93:VAL:HG21	1.90	0.53
1:G:260:TYR:O	1:G:264:VAL:HG13	2.09	0.53
1:G:379:ILE:HG12	1:H:291:LEU:HD22	1.90	0.53
1:H:149:ARG:CG	1:H:156:VAL:CG1	2.87	0.53
1:A:156:VAL:O	1:A:156:VAL:HG13	2.09	0.53
1:E:25:PHE:CD2	1:E:54:LEU:HD22	2.43	0.53
1:H:276:PRO:HD2	1:H:279:LYS:HB2	1.90	0.53
1:H:35:ARG:CD	1:I:203:ARG:NH1	2.72	0.53
1:C:110:GLU:HG2	1:C:114:ARG:NH1	2.24	0.53
1:F:262:GLU:OE2	1:F:349:TYR:O	2.26	0.53
1:H:12:THR:OG1	1:H:15:GLU:HG3	2.09	0.53
1:I:23:ARG:O	1:I:27:GLU:HB2	2.08	0.53
1:I:35:ARG:NH1	1:I:347:LEU:O	2.42	0.53
1:C:125:MET:HG2	1:C:125:MET:O	2.08	0.52
1:C:12:THR:HG1	1:C:15:GLU:HG3	1.70	0.52
1:C:35:ARG:CD	1:E:203:ARG:NH2	2.68	0.52
1:G:16:LYS:O	1:G:20:LYS:HG2	2.08	0.52
1:G:48:ILE:HB	1:G:49:PRO:HD3	1.90	0.52
1:H:337:ARG:HG3	1:H:355:MET:HE3	1.91	0.52
1:I:163:TRP:CZ3	1:I:201:VAL:HG11	2.43	0.52
1:F:279:LYS:HB2	1:I:382:LEU:HD13	1.91	0.52
1:A:337:ARG:HB2	1:A:355:MET:HE3	1.91	0.52
1:D:253:MET:HE3	1:D:256:LEU:HD13	1.91	0.52
1:E:48:ILE:HB	1:E:49:PRO:HD3	1.91	0.52
1:H:122:ARG:HG2	3:H:7024:HOH:O	2.09	0.52
1:H:205:MET:HE1	1:I:205:MET:CE	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:156:VAL:HG21	1:I:219:GLU:OE2	2.10	0.52
1:F:167:GLY:HA3	1:F:213:SER:HB2	1.90	0.52
1:G:57:LEU:HG	1:G:96:GLN:HG2	1.90	0.52
1:I:314:THR:OG1	1:I:317:GLN:HG3	2.09	0.52
1:A:349:TYR:O	1:A:350:HIS:HB2	2.09	0.52
1:C:109:SER:OG	1:C:112:GLN:HG3	2.09	0.52
1:C:110:GLU:CG	1:C:114:ARG:NH1	2.73	0.52
1:C:349:TYR:O	1:C:350:HIS:HB2	2.10	0.52
1:D:237:PRO:O	1:D:240:CYS:HB2	2.09	0.52
1:E:237:PRO:O	1:E:240:CYS:HB2	2.09	0.52
1:A:78:ILE:HD11	1:A:93:VAL:HG11	1.92	0.52
1:F:205:MET:HE1	1:G:205:MET:CE	2.40	0.52
1:E:314:THR:OG1	1:E:317:GLN:HG3	2.10	0.52
1:I:163:TRP:HZ3	1:I:201:VAL:HG11	1.75	0.52
1:G:282:LEU:HG	1:I:281:GLN:HE21	1.75	0.52
1:D:334:ARG:HA	1:D:355:MET:HE3	1.91	0.52
1:F:248:ILE:CD1	1:F:365:GLU:HG3	2.39	0.52
1:F:63:PRO:HA	1:F:67:GLY:O	2.10	0.52
1:G:109:SER:OG	1:G:112:GLN:HG3	2.09	0.52
1:F:281:GLN:NE2	1:H:282:LEU:H	2.07	0.52
1:I:260:TYR:HA	1:I:290:MET:HE1	1.92	0.52
1:C:176:TRP:CE2	1:C:237:PRO:HB3	2.44	0.52
1:C:272:THR:HG21	1:C:273:PHE:CE1	2.45	0.52
1:C:346:THR:C	1:C:348:GLU:H	2.13	0.52
1:A:346:THR:HG23	1:D:203:ARG:HB2	1.92	0.52
1:A:78:ILE:HD12	1:A:82:LEU:CD1	2.39	0.52
1:C:234:LEU:HD22	1:C:238:LEU:CG	2.36	0.52
1:F:15:GLU:OE2	1:F:73:ALA:HB3	2.10	0.52
1:G:272:THR:CG2	1:G:273:PHE:H	2.11	0.52
1:F:359:GLU:HG3	1:G:337:ARG:NH2	2.25	0.52
1:H:205:MET:CE	1:I:205:MET:HE2	2.40	0.52
1:F:346:THR:HG22	1:F:348:GLU:N	2.23	0.52
1:F:349:TYR:O	1:F:350:HIS:HB2	2.10	0.52
1:D:253:MET:CE	1:D:294:HIS:CA	2.74	0.51
1:D:35:ARG:NH1	1:D:347:LEU:O	2.42	0.51
1:A:234:LEU:O	1:A:238:LEU:HG	2.10	0.51
1:C:361:VAL:HG22	1:C:364:TYR:CZ	2.45	0.51
1:F:171:HIS:O	1:F:190:PRO:HA	2.11	0.51
1:F:272:THR:HG22	1:F:273:PHE:HD1	1.74	0.51
1:F:270:ARG:HB3	1:F:277:LEU:HD22	1.93	0.51
1:F:205:MET:CE	1:G:205:MET:HE2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:234:LEU:HD22	1:G:238:LEU:HG	1.92	0.51
1:H:163:TRP:HZ3	1:H:201:VAL:HG11	1.74	0.51
1:H:39:GLU:HB3	1:H:347:LEU:CD1	2.40	0.51
1:I:231:ALA:O	1:I:232:LEU:HD12	2.10	0.51
1:I:63:PRO:HA	1:I:67:GLY:O	2.11	0.51
1:E:334:ARG:HA	1:E:355:MET:HE1	1.92	0.51
1:H:234:LEU:HD22	1:H:238:LEU:HG	1.91	0.51
1:H:234:LEU:O	1:H:238:LEU:HG	2.10	0.51
1:A:262:GLU:OE1	1:A:349:TYR:O	2.29	0.51
1:C:310:GLU:OE1	1:C:312:LYS:CE	2.59	0.51
1:C:297:GLY:HA2	1:C:325:ASN:HD21	1.75	0.51
1:D:157:LEU:HD13	1:D:222:VAL:CG2	2.39	0.51
1:E:335:MET:O	1:E:339:ILE:HG13	2.09	0.51
1:F:253:MET:CE	1:F:256:LEU:HD13	2.41	0.51
1:H:7:LEU:HD11	1:H:299:LEU:CD2	2.39	0.51
1:C:242:THR:HG22	1:C:318:VAL:HG21	1.93	0.51
1:E:383:ASN:HD22	1:E:383:ASN:C	2.13	0.51
1:G:120:LEU:HD23	1:G:125:MET:HG2	1.93	0.51
1:G:260:TYR:HA	1:G:290:MET:HE1	1.93	0.51
1:C:78:ILE:HD12	1:C:82:LEU:HD12	1.92	0.51
1:D:126:VAL:H	1:D:171:HIS:CE1	2.29	0.51
1:D:272:THR:CG2	1:D:273:PHE:CE1	2.94	0.51
1:E:146:THR:HA	1:E:159:GLY:HA3	1.92	0.51
1:E:49:PRO:HA	3:E:4060:HOH:O	2.09	0.51
1:I:280:LYS:O	1:I:283:VAL:HG22	2.11	0.51
1:A:275:GLU:HG3	1:A:280:LYS:NZ	2.26	0.51
1:A:36:ASP:O	1:A:40:GLU:HG2	2.11	0.51
1:D:52:ALA:O	1:D:53:GLU:C	2.49	0.51
1:H:335:MET:O	1:H:339:ILE:HG13	2.11	0.51
1:C:56:PHE:O	1:C:59:PRO:HD3	2.11	0.51
1:E:110:GLU:O	1:E:114:ARG:HG3	2.10	0.51
1:G:253:MET:SD	1:G:297:GLY:HA3	2.51	0.51
1:I:130:GLY:HA2	1:I:164:ILE:HD12	1.92	0.51
1:A:260:TYR:HA	1:A:290:MET:CE	2.41	0.50
1:C:90:ARG:NH2	1:C:364:TYR:OH	2.40	0.50
1:D:82:LEU:HD11	1:D:93:VAL:HG21	1.92	0.50
1:G:262:GLU:OE2	1:G:349:TYR:O	2.28	0.50
1:G:367:THR:OG1	1:G:370:VAL:HG13	2.11	0.50
1:C:14:GLU:O	1:C:18:VAL:HG13	2.11	0.50
1:F:96:GLN:O	1:F:101:MET:HG3	2.11	0.50
1:D:144:MET:O	1:D:178:LYS:HE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:GLY:HA3	1:D:213:SER:HB2	1.92	0.50
1:F:300:LEU:HD22	1:I:5:TYR:CE2	2.47	0.50
1:F:48:ILE:HB	1:F:49:PRO:HD3	1.93	0.50
1:I:140:PRO:HG2	1:I:141:TYR:H	1.75	0.50
1:D:162:MET:CE	1:D:162:MET:CA	2.90	0.50
1:E:125:MET:HE1	1:E:172:LEU:HD22	1.94	0.50
1:F:281:GLN:NE2	1:H:282:LEU:HG	2.26	0.50
1:G:259:VAL:HG23	1:G:290:MET:CE	2.42	0.50
1:I:156:VAL:O	1:I:156:VAL:HG13	2.11	0.50
1:I:262:GLU:OE1	1:I:349:TYR:O	2.29	0.50
1:A:270:ARG:HB3	1:A:277:LEU:HD23	1.93	0.50
1:C:57:LEU:CB	1:C:101:MET:HE1	2.34	0.50
1:E:34:ILE:HG12	1:E:86:ASP:HB2	1.94	0.50
1:E:337:ARG:CB	1:E:355:MET:CE	2.90	0.50
1:F:281:GLN:HE21	1:H:282:LEU:HG	1.76	0.50
1:G:367:THR:O	1:G:370:VAL:HG22	2.12	0.50
1:H:179:ASP:OD2	1:H:183:GLU:HB3	2.12	0.50
1:H:367:THR:OG1	1:H:370:VAL:HG13	2.12	0.50
1:I:7:LEU:HD13	1:I:10:LEU:CD1	2.42	0.50
1:D:314:THR:OG1	1:D:317:GLN:HG3	2.12	0.50
1:F:337:ARG:CB	1:F:355:MET:CE	2.90	0.50
1:H:35:ARG:CG	1:H:35:ARG:HH11	2.25	0.50
1:D:310:GLU:HG3	1:D:312:LYS:HE2	1.93	0.50
1:E:96:GLN:HG3	1:E:101:MET:HE2	1.94	0.50
1:F:118:PRO:O	1:F:122:ARG:HG3	2.11	0.50
1:F:373:LEU:HB3	1:F:385:PHE:CZ	2.46	0.50
1:I:149:ARG:NH2	3:I:8026:HOH:O	2.10	0.50
1:A:23:ARG:O	1:A:27:GLU:HB2	2.11	0.50
1:C:233:GLY:O	1:C:237:PRO:HD2	2.12	0.50
1:E:286:LYS:O	1:E:290:MET:HG3	2.12	0.50
1:C:39:GLU:HG3	1:C:347:LEU:CD1	2.42	0.49
1:D:96:GLN:HG3	1:D:101:MET:CE	2.41	0.49
1:A:205:MET:CE	1:D:205:MET:CE	2.90	0.49
1:F:271:SER:HB2	1:F:276:PRO:HA	1.94	0.49
2:F:5001:FAD:H4B	1:G:339:ILE:O	2.12	0.49
1:G:58:GLY:HA3	1:G:101:MET:SD	2.51	0.49
1:H:346:THR:C	1:H:348:GLU:H	2.16	0.49
1:I:140:PRO:CG	1:I:141:TYR:N	2.74	0.49
1:G:272:THR:HG21	1:G:273:PHE:CE1	2.47	0.49
1:H:7:LEU:HD13	1:H:10:LEU:CD1	2.42	0.49
1:C:262:GLU:CD	1:C:349:TYR:O	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:144:MET:O	1:H:178:LYS:HE2	2.12	0.49
1:H:359:GLU:CG	1:I:337:ARG:NE	2.75	0.49
1:I:58:GLY:N	1:I:101:MET:HE1	2.27	0.49
1:G:337:ARG:CG	1:G:355:MET:HE1	2.40	0.49
1:G:56:PHE:O	1:G:59:PRO:HD3	2.12	0.49
1:G:63:PRO:HA	1:G:67:GLY:O	2.12	0.49
1:C:306:ARG:O	1:C:310:GLU:HG2	2.12	0.49
1:E:63:PRO:HA	1:E:67:GLY:O	2.12	0.49
1:E:253:MET:HE1	1:E:294:HIS:CA	2.09	0.49
1:E:346:THR:HG22	1:E:348:GLU:N	2.25	0.49
1:F:179:ASP:OD2	1:F:183:GLU:HB3	2.12	0.49
1:I:253:MET:CE	1:I:294:HIS:CA	2.72	0.49
1:I:48:ILE:HB	1:I:49:PRO:HD3	1.94	0.49
1:I:7:LEU:CD1	1:I:10:LEU:HD12	2.42	0.49
2:A:1001:FAD:H4B	1:D:339:ILE:O	2.12	0.49
1:A:156:VAL:HG21	1:A:219:GLU:OE2	2.13	0.49
1:A:63:PRO:HA	1:A:67:GLY:O	2.12	0.49
1:D:291:LEU:HD22	1:E:379:ILE:HG12	1.95	0.49
1:C:345:ILE:HB	1:E:206:SER:HB3	1.93	0.49
1:G:205:MET:HE3	1:G:205:MET:HA	1.95	0.49
1:G:346:THR:C	1:G:348:GLU:H	2.15	0.49
1:H:275:GLU:HG2	1:H:280:LYS:NZ	2.27	0.49
1:D:256:LEU:O	1:D:256:LEU:HD23	2.13	0.49
1:D:275:GLU:HB2	1:D:276:PRO:CD	2.42	0.49
1:E:279:LYS:HG2	1:E:279:LYS:O	2.11	0.49
1:F:203:ARG:HG2	1:G:35:ARG:HH22	1.77	0.49
1:E:262:GLU:OE2	1:E:349:TYR:O	2.30	0.49
1:F:130:GLY:HA2	1:F:164:ILE:HD12	1.95	0.49
1:F:173:ALA:HB1	1:F:175:ILE:CD1	2.42	0.49
1:F:272:THR:CG2	1:F:273:PHE:CD1	2.96	0.49
1:A:163:TRP:CZ3	1:A:201:VAL:HG11	2.48	0.49
1:C:207:LEU:H	1:C:357:ASN:ND2	2.11	0.49
1:E:39:GLU:HG2	1:E:347:LEU:CD1	2.43	0.49
1:F:376:GLY:HA3	1:I:284:GLN:NE2	2.28	0.49
1:I:383:ASN:HD22	1:I:383:ASN:C	2.16	0.49
1:H:205:MET:HE1	1:I:205:MET:HE2	1.94	0.48
1:C:262:GLU:OE1	1:C:349:TYR:O	2.30	0.48
1:C:35:ARG:HH11	1:C:35:ARG:CG	2.26	0.48
1:D:275:GLU:HG2	1:D:280:LYS:NZ	2.28	0.48
1:E:147:ARG:HH11	1:E:147:ARG:HG2	1.78	0.48
1:E:367:THR:OG1	1:E:370:VAL:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:5031:HOH:O	1:G:346:THR:HG23	2.11	0.48
1:G:349:TYR:O	1:G:350:HIS:HB2	2.13	0.48
1:D:8:GLU:HG2	1:D:11:LEU:HD12	1.95	0.48
1:C:176:TRP:CD2	1:C:237:PRO:HB3	2.48	0.48
1:D:272:THR:C	1:D:274:GLY:H	2.17	0.48
1:F:163:TRP:HZ3	1:F:201:VAL:HG11	1.78	0.48
1:G:291:LEU:HD22	1:H:379:ILE:CG1	2.43	0.48
1:I:179:ASP:OD2	1:I:183:GLU:HB3	2.13	0.48
1:I:82:LEU:HD11	1:I:93:VAL:HG21	1.95	0.48
1:F:279:LYS:O	1:I:384:ALA:HB2	2.12	0.48
1:G:14:GLU:HB2	3:G:6021:HOH:O	2.14	0.48
1:G:337:ARG:CB	1:G:355:MET:HE1	2.42	0.48
1:I:110:GLU:O	1:I:114:ARG:HG3	2.13	0.48
1:C:39:GLU:HG3	1:C:347:LEU:HD12	1.96	0.48
1:D:346:THR:C	1:D:348:GLU:H	2.17	0.48
1:F:250:TRP:CE2	1:F:301:ALA:HB1	2.49	0.48
1:G:281:GLN:NE2	1:I:282:LEU:H	2.11	0.48
1:I:78:ILE:HD12	1:I:82:LEU:CD1	2.42	0.48
1:A:57:LEU:HB3	1:A:101:MET:CE	2.43	0.48
1:D:110:GLU:O	1:D:114:ARG:HG3	2.14	0.48
1:D:54:LEU:HD12	1:D:54:LEU:N	2.29	0.48
1:A:163:TRP:HZ3	1:A:201:VAL:HG11	1.78	0.48
1:C:50:ARG:NH1	1:C:53:GLU:OE1	2.40	0.48
1:D:179:ASP:OD2	1:D:183:GLU:HB3	2.13	0.48
1:C:281:GLN:NE2	1:D:282:LEU:H	2.11	0.48
1:D:7:LEU:CD1	1:D:10:LEU:HD12	2.44	0.48
1:E:144:MET:O	1:E:178:LYS:HE2	2.13	0.48
1:E:162:MET:HE2	1:E:163:TRP:N	2.06	0.48
1:E:232:LEU:HD12	1:E:233:GLY:N	2.28	0.48
1:F:163:TRP:CZ3	1:F:201:VAL:HG11	2.48	0.48
1:F:58:GLY:N	1:F:59:PRO:CD	2.76	0.48
1:H:260:TYR:O	1:H:264:VAL:HG13	2.14	0.48
1:H:46:HIS:O	1:H:49:PRO:HD2	2.13	0.48
1:I:167:GLY:HA3	1:I:213:SER:HB2	1.95	0.48
1:H:35:ARG:HD3	1:I:203:ARG:NH1	2.29	0.48
1:I:262:GLU:OE2	1:I:349:TYR:O	2.31	0.48
1:A:144:MET:SD	1:A:178:LYS:HG3	2.54	0.48
1:C:270:ARG:HH12	1:E:136:GLY:HA2	1.79	0.48
1:C:35:ARG:NH1	1:C:347:LEU:O	2.47	0.48
1:F:149:ARG:HG2	1:F:156:VAL:CG1	2.41	0.48
1:F:253:MET:CE	1:F:294:HIS:CA	2.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:260:TYR:O	1:I:264:VAL:HG13	2.14	0.48
1:A:234:LEU:HD22	1:A:238:LEU:HG	1.96	0.47
1:D:163:TRP:CZ3	1:D:201:VAL:HG11	2.49	0.47
1:E:323:ARG:HD3	1:E:324:GLN:OE1	2.14	0.47
1:E:91:SER:O	1:E:95:VAL:HG23	2.13	0.47
1:A:102:TYR:N	1:A:103:PRO:CD	2.75	0.47
1:C:234:LEU:O	1:C:238:LEU:HG	2.14	0.47
1:C:349:TYR:O	1:C:351:ALA:N	2.44	0.47
1:G:383:ASN:C	1:G:383:ASN:HD22	2.17	0.47
1:G:57:LEU:CA	1:G:101:MET:HE1	2.44	0.47
1:G:39:GLU:HG3	1:G:347:LEU:HD12	1.96	0.47
1:I:237:PRO:O	1:I:240:CYS:HB2	2.14	0.47
1:A:50:ARG:O	1:A:54:LEU:HD13	2.15	0.47
1:A:78:ILE:HD12	1:A:82:LEU:HD12	1.96	0.47
1:E:262:GLU:OE1	1:E:349:TYR:O	2.32	0.47
1:E:350:HIS:N	3:E:4049:HOH:O	2.47	0.47
1:G:378:GLU:HG2	3:G:6080:HOH:O	2.14	0.47
1:H:20:LYS:HE2	1:H:20:LYS:HA	1.94	0.47
1:A:110:GLU:OE2	1:A:114:ARG:NH2	2.48	0.47
1:A:205:MET:CE	1:D:205:MET:HE2	2.45	0.47
1:D:162:MET:HE3	1:D:162:MET:CA	2.38	0.47
1:H:260:TYR:HA	1:H:290:MET:HE1	1.96	0.47
1:E:147:ARG:NH1	1:E:147:ARG:HG2	2.30	0.47
1:E:95:VAL:HG11	1:E:166:ASN:HD22	1.79	0.47
1:F:367:THR:OG1	1:F:370:VAL:HG13	2.14	0.47
1:H:337:ARG:CG	1:H:355:MET:HE3	2.44	0.47
1:A:346:THR:HA	1:D:203:ARG:O	2.15	0.47
1:A:337:ARG:HB3	1:A:355:MET:HE1	1.94	0.47
1:A:91:SER:O	1:A:95:VAL:HG23	2.15	0.47
1:A:281:GLN:NE2	1:E:282:LEU:H	2.13	0.47
1:A:262:GLU:OE2	1:A:349:TYR:O	2.32	0.47
1:A:284:GLN:NE2	1:C:376:GLY:HA3	2.29	0.47
1:C:117:LEU:HB2	1:C:118:PRO:HD3	1.97	0.47
1:C:118:PRO:O	1:C:122:ARG:HG3	2.15	0.47
1:C:46:HIS:O	1:C:49:PRO:HD2	2.15	0.47
1:E:183:GLU:HG2	3:E:4026:HOH:O	2.14	0.47
1:F:383:ASN:C	1:F:383:ASN:HD22	2.18	0.47
1:H:96:GLN:HG3	1:H:101:MET:HE2	1.97	0.47
1:H:183:GLU:N	3:H:7050:HOH:O	2.48	0.47
1:H:323:ARG:HD3	1:H:324:GLN:OE1	2.15	0.47
1:A:50:ARG:O	1:A:54:LEU:CD1	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:THR:HG21	1:C:273:PHE:CD1	2.50	0.47
1:D:35:ARG:HH11	1:D:35:ARG:CG	2.27	0.47
1:F:337:ARG:HB2	1:F:355:MET:CE	2.45	0.47
1:G:20:LYS:HE2	1:G:20:LYS:HA	1.96	0.47
1:G:382:LEU:CD1	1:H:279:LYS:HB2	2.40	0.47
1:C:20:LYS:HE2	1:C:20:LYS:HA	1.97	0.47
1:F:58:GLY:CA	1:F:101:MET:SD	3.01	0.47
1:H:15:GLU:OE2	1:H:73:ALA:HB3	2.15	0.47
1:I:126:VAL:HG13	1:I:169:LEU:O	2.14	0.47
1:I:257:GLU:O	1:I:261:GLU:HB2	2.14	0.47
1:A:203:ARG:O	1:D:346:THR:HA	2.15	0.46
1:C:226:LEU:HA	1:C:226:LEU:HD12	1.62	0.46
1:E:107:TYR:HA	1:E:230:LYS:HB2	1.97	0.46
2:C:2001:FAD:HM81	1:E:342:GLY:HA2	1.95	0.46
1:F:337:ARG:HB2	1:F:355:MET:HE3	1.97	0.46
1:H:34:ILE:HG12	1:H:86:ASP:HB2	1.96	0.46
1:I:110:GLU:HG3	1:I:114:ARG:CZ	2.45	0.46
1:F:34:ILE:HG12	1:F:86:ASP:HB2	1.98	0.46
1:I:367:THR:O	1:I:370:VAL:HG22	2.14	0.46
1:D:130:GLY:HA2	1:D:164:ILE:HD12	1.98	0.46
1:F:110:GLU:O	1:F:114:ARG:HG3	2.16	0.46
1:G:34:ILE:HG12	1:G:86:ASP:HB2	1.98	0.46
1:A:256:LEU:HD23	1:A:256:LEU:O	2.16	0.46
2:C:2001:FAD:C8A	1:E:277:LEU:HD11	2.45	0.46
1:C:272:THR:CG2	1:C:273:PHE:CE1	2.99	0.46
1:C:326:VAL:HG11	1:C:362:TYR:HA	1.96	0.46
1:D:259:VAL:HG23	1:D:290:MET:CE	2.46	0.46
1:E:337:ARG:HG3	1:E:355:MET:HE3	1.97	0.46
1:E:35:ARG:NH1	1:E:35:ARG:CB	2.72	0.46
1:F:264:VAL:HG12	1:F:287:LEU:HD22	1.98	0.46
1:G:116:PHE:CD1	1:G:125:MET:HE1	2.51	0.46
1:G:289:GLU:HB2	3:H:7079:HOH:O	2.15	0.46
1:A:323:ARG:HD3	1:A:324:GLN:OE1	2.16	0.46
1:D:7:LEU:HD12	1:D:10:LEU:HD12	1.96	0.46
1:E:14:GLU:O	1:E:18:VAL:HG13	2.15	0.46
1:G:320:LEU:HD11	1:H:292:ALA:CB	2.45	0.46
1:H:367:THR:O	1:H:370:VAL:HG22	2.16	0.46
1:A:383:ASN:C	1:A:383:ASN:HD22	2.19	0.46
1:C:50:ARG:O	1:C:54:LEU:HD13	2.15	0.46
1:G:271:SER:HB2	1:G:276:PRO:HA	1.97	0.46
1:G:337:ARG:HG3	1:G:355:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:20:LYS:HE2	1:I:20:LYS:HA	1.97	0.46
1:E:118:PRO:O	1:E:122:ARG:HG3	2.16	0.46
1:E:130:GLY:HA2	1:E:164:ILE:HD12	1.97	0.46
1:F:277:LEU:HA	1:F:277:LEU:HD12	1.71	0.46
1:G:234:LEU:O	1:G:238:LEU:HG	2.16	0.46
1:G:36:ASP:O	1:G:40:GLU:CG	2.42	0.46
1:H:156:VAL:HG21	1:H:219:GLU:OE2	2.16	0.46
1:H:272:THR:O	1:H:274:GLY:N	2.46	0.46
1:H:346:THR:CG2	3:I:8048:HOH:O	2.53	0.46
1:A:144:MET:O	1:A:178:LYS:HE2	2.16	0.46
1:A:167:GLY:HA3	1:A:213:SER:HB2	1.98	0.46
1:A:337:ARG:HE	1:D:359:GLU:CG	2.29	0.46
1:C:176:TRP:CZ3	1:C:237:PRO:HD3	2.51	0.46
1:D:367:THR:O	1:D:370:VAL:HG22	2.16	0.46
1:F:50:ARG:O	1:F:54:LEU:HD13	2.16	0.46
1:H:226:LEU:HA	1:H:226:LEU:HD12	1.75	0.46
1:D:162:MET:CE	1:D:163:TRP:N	2.56	0.46
1:D:377:ARG:HD2	3:D:3059:HOH:O	2.15	0.46
1:D:48:ILE:HB	1:D:49:PRO:HD2	1.98	0.46
1:F:170:ALA:O	1:F:191:THR:HG21	2.15	0.46
1:G:125:MET:CE	1:G:172:LEU:HD22	2.45	0.46
1:I:103:PRO:HB3	1:I:240:CYS:SG	2.55	0.46
1:I:346:THR:C	1:I:348:GLU:H	2.18	0.46
1:A:272:THR:O	1:A:273:PHE:HB2	2.15	0.45
1:F:35:ARG:CZ	1:F:39:GLU:OE1	2.63	0.45
1:G:147:ARG:HD3	1:G:147:ARG:HA	1.76	0.45
1:H:156:VAL:O	1:H:156:VAL:HG13	2.15	0.45
1:D:277:LEU:HA	1:D:277:LEU:HD12	1.71	0.45
1:E:207:LEU:HD22	1:E:360:THR:HG21	1.97	0.45
1:G:373:LEU:HB3	1:G:385:PHE:CZ	2.51	0.45
1:H:207:LEU:HD22	1:H:360:THR:HG21	1.99	0.45
1:H:96:GLN:HG3	1:H:101:MET:CE	2.47	0.45
1:D:96:GLN:O	1:D:101:MET:HG3	2.16	0.45
1:D:163:TRP:HZ3	1:D:201:VAL:HG11	1.81	0.45
1:D:78:ILE:HD12	1:D:82:LEU:CD1	2.46	0.45
1:E:226:LEU:HD12	1:E:226:LEU:HA	1.66	0.45
1:E:277:LEU:O	1:E:280:LYS:HG2	2.17	0.45
1:E:310:GLU:OE1	1:E:312:LYS:CE	2.64	0.45
1:E:132:THR:OG1	2:E:4001:FAD:H1'1	2.16	0.45
1:F:323:ARG:HD3	1:F:324:GLN:OE1	2.16	0.45
1:H:262:GLU:OE2	1:H:349:TYR:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:91:SER:O	1:H:95:VAL:HG23	2.17	0.45
1:A:80:TYR:HA	1:A:251:GLY:HA2	1.97	0.45
1:C:277:LEU:HD12	1:C:277:LEU:HA	1.74	0.45
1:D:8:GLU:C	1:D:10:LEU:N	2.68	0.45
1:E:162:MET:HA	1:E:162:MET:CE	2.42	0.45
1:G:21:ALA:HA	1:G:24:ARG:NH1	2.31	0.45
1:G:23:ARG:O	1:G:27:GLU:HB2	2.16	0.45
1:H:280:LYS:HB2	1:H:283:VAL:CG1	2.45	0.45
1:A:48:ILE:HB	1:A:49:PRO:CD	2.47	0.45
1:C:47:LEU:HA	1:C:47:LEU:HD12	1.76	0.45
1:C:50:ARG:O	1:C:54:LEU:CD1	2.64	0.45
1:E:346:THR:C	1:E:348:GLU:H	2.20	0.45
1:F:228:LEU:HA	1:F:229:PRO:HD2	1.87	0.45
1:F:260:TYR:HA	1:F:290:MET:HE1	1.97	0.45
1:G:110:GLU:OE2	1:G:114:ARG:NH2	2.49	0.45
1:D:244:ALA:HB1	1:D:365:GLU:OE2	2.16	0.45
1:E:349:TYR:O	1:E:351:ALA:N	2.46	0.45
1:H:103:PRO:HB3	1:H:240:CYS:SG	2.55	0.45
1:A:257:GLU:O	1:A:261:GLU:HB2	2.15	0.45
1:C:116:PHE:HD1	1:C:125:MET:HE1	1.81	0.45
1:C:197:GLN:HA	1:C:197:GLN:NE2	2.29	0.45
1:F:8:GLU:HA	1:F:11:LEU:CD1	2.46	0.45
1:G:156:VAL:HA	1:G:220:VAL:O	2.17	0.45
1:G:167:GLY:HA3	1:G:213:SER:HB2	1.98	0.45
1:G:342:GLY:O	1:G:345:ILE:HG12	2.17	0.45
1:I:259:VAL:HG23	1:I:290:MET:CE	2.46	0.45
1:A:282:LEU:H	1:E:281:GLN:HE22	1.65	0.45
1:A:7:LEU:HD12	1:A:10:LEU:HD12	1.99	0.45
1:C:150:ARG:HB2	1:C:155:TRP:CE2	2.52	0.45
1:C:2:LEU:HD23	1:C:294:HIS:CD2	2.51	0.45
1:D:275:GLU:HG2	1:D:280:LYS:HZ2	1.81	0.45
3:A:1075:HOH:O	1:D:338:ASP:HB2	2.16	0.45
1:E:36:ASP:O	1:E:39:GLU:HB2	2.16	0.45
1:F:286:LYS:O	1:F:290:MET:HG3	2.15	0.45
1:F:328:LYS:HZ1	1:I:296:GLU:CD	2.18	0.45
1:G:197:GLN:NE2	1:G:197:GLN:HA	2.29	0.45
3:H:7042:HOH:O	1:I:203:ARG:CD	2.55	0.45
1:I:35:ARG:CD	3:I:8009:HOH:O	2.56	0.45
1:C:346:THR:CG2	3:E:4040:HOH:O	2.61	0.45
1:E:162:MET:O	1:E:163:TRP:C	2.54	0.45
1:E:179:ASP:OD2	1:E:183:GLU:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:THR:C	1:E:274:GLY:N	2.69	0.45
1:C:206:SER:HB3	1:E:345:ILE:HB	1.98	0.45
1:F:260:TYR:HA	1:F:290:MET:CE	2.47	0.45
1:G:14:GLU:O	1:G:18:VAL:HG13	2.17	0.45
1:H:58:GLY:N	1:H:59:PRO:CD	2.80	0.45
1:C:125:MET:CE	1:C:172:LEU:HD22	2.46	0.45
1:E:326:VAL:HG11	1:E:362:TYR:HA	1.98	0.45
1:I:80:TYR:HA	1:I:251:GLY:HA2	1.99	0.45
1:A:197:GLN:NE2	1:A:197:GLN:HA	2.30	0.44
1:C:136:GLY:HA2	1:E:270:ARG:HH12	1.82	0.44
1:C:31:LEU:HB3	1:C:32:PRO:HD3	1.98	0.44
1:C:63:PRO:HA	1:C:67:GLY:O	2.17	0.44
1:D:63:PRO:HA	1:D:67:GLY:O	2.17	0.44
1:E:264:VAL:HG12	1:E:287:LEU:HD22	2.00	0.44
1:F:20:LYS:HE2	1:F:20:LYS:HA	1.98	0.44
1:F:283:VAL:HG23	1:F:284:GLN:N	2.31	0.44
1:G:208:ARG:HA	3:G:6064:HOH:O	2.16	0.44
1:H:190:PRO:O	1:H:193:THR:CG2	2.64	0.44
1:A:14:GLU:O	1:A:18:VAL:HG13	2.17	0.44
1:C:34:ILE:HG12	1:C:86:ASP:HB2	1.98	0.44
1:E:171:HIS:O	1:E:190:PRO:HA	2.16	0.44
1:F:346:THR:C	1:F:348:GLU:H	2.20	0.44
1:G:227:ARG:O	1:G:229:PRO:HD3	2.17	0.44
1:G:228:LEU:HA	1:G:228:LEU:HD12	1.86	0.44
1:G:364:TYR:C	1:G:364:TYR:CD1	2.91	0.44
1:I:14:GLU:O	1:I:18:VAL:HG13	2.17	0.44
1:A:270:ARG:HB3	1:A:277:LEU:CD2	2.47	0.44
1:A:280:LYS:HE2	2:D:3001:FAD:N6A	2.33	0.44
1:A:39:GLU:HG3	1:A:347:LEU:HD12	1.99	0.44
1:F:346:THR:HG23	3:G:6039:HOH:O	2.14	0.44
1:G:110:GLU:O	1:G:114:ARG:HG3	2.17	0.44
1:G:256:LEU:O	1:G:256:LEU:HD23	2.16	0.44
1:H:205:MET:CE	1:I:205:MET:HE1	2.47	0.44
1:H:272:THR:HG23	1:H:273:PHE:CD1	2.49	0.44
3:H:7064:HOH:O	1:I:338:ASP:HB2	2.18	0.44
1:A:339:ILE:O	2:D:3001:FAD:H4B	2.17	0.44
1:E:349:TYR:O	1:E:350:HIS:HB2	2.17	0.44
1:F:367:THR:O	1:F:370:VAL:HG22	2.17	0.44
1:G:83:GLU:OE1	1:G:251:GLY:HA3	2.17	0.44
1:A:272:THR:HG22	1:A:272:THR:O	2.16	0.44
1:C:337:ARG:O	1:C:337:ARG:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:383:ASN:O	1:I:279:LYS:HE3	2.18	0.44
1:G:35:ARG:HH12	1:G:39:GLU:CD	2.20	0.44
1:H:125:MET:HE1	1:H:172:LEU:CD2	2.36	0.44
1:I:362:TYR:CE1	1:I:368:HIS:HB2	2.53	0.44
1:I:39:GLU:HG2	1:I:347:LEU:CD1	2.47	0.44
1:A:132:THR:OG1	2:A:1001:FAD:H1'1	2.17	0.44
1:C:222:VAL:HG12	1:C:223:PRO:HD2	1.98	0.44
1:C:375:LEU:O	1:C:379:ILE:HG13	2.17	0.44
1:D:226:LEU:HA	1:D:226:LEU:HD12	1.70	0.44
1:D:23:ARG:HE	1:D:81:GLU:CD	2.21	0.44
1:E:31:LEU:HB3	1:E:32:PRO:HD3	1.99	0.44
1:G:96:GLN:HG3	1:G:101:MET:HE2	2.00	0.44
1:I:234:LEU:O	1:I:238:LEU:HG	2.17	0.44
1:C:184:VAL:HG23	3:C:2017:HOH:O	2.16	0.44
1:C:35:ARG:CG	1:E:203:ARG:NH2	2.81	0.44
1:D:126:VAL:HG13	1:D:169:LEU:O	2.17	0.44
1:D:241:LEU:O	1:D:245:ARG:HG3	2.17	0.44
1:E:260:TYR:HA	1:E:290:MET:HE1	2.00	0.44
1:E:49:PRO:CA	3:E:4060:HOH:O	2.66	0.44
1:F:25:PHE:CD2	1:F:54:LEU:HD22	2.53	0.44
1:H:275:GLU:HG2	1:H:280:LYS:HZ1	1.81	0.44
1:G:299:LEU:CD1	1:H:300:LEU:HD23	2.48	0.44
1:A:100:VAL:C	1:A:103:PRO:CD	2.81	0.44
1:A:359:GLU:CG	1:D:337:ARG:HE	2.29	0.44
1:C:270:ARG:O	1:C:271:SER:HB3	2.18	0.44
1:C:48:ILE:HB	1:C:49:PRO:HD3	1.99	0.44
1:D:8:GLU:C	1:D:10:LEU:H	2.21	0.44
1:F:57:LEU:CB	1:F:101:MET:HE1	2.22	0.44
1:G:203:ARG:HB2	3:G:6039:HOH:O	2.17	0.44
1:H:162:MET:SD	1:H:214:GLU:HG3	2.58	0.44
1:H:48:ILE:HB	1:H:49:PRO:HD3	2.00	0.44
1:I:34:ILE:HG12	1:I:86:ASP:HB2	1.99	0.44
1:A:163:TRP:O	2:A:1001:FAD:C4X	2.66	0.44
1:A:253:MET:CE	1:A:256:LEU:HD13	2.46	0.44
1:C:23:ARG:O	1:C:27:GLU:HB2	2.18	0.44
1:C:58:GLY:N	1:C:59:PRO:CD	2.81	0.44
1:D:146:THR:HG22	1:D:177:ALA:HB2	2.00	0.44
1:E:198:ALA:HA	1:E:214:GLU:O	2.17	0.44
2:C:2001:FAD:H4B	1:E:339:ILE:O	2.18	0.44
1:F:272:THR:HG22	1:F:273:PHE:H	1.75	0.44
1:G:231:ALA:C	1:G:232:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:282:LEU:HG	1:I:281:GLN:NE2	2.32	0.44
1:I:58:GLY:HA3	1:I:101:MET:SD	2.58	0.44
1:A:62:PRO:HA	1:A:63:PRO:HD3	1.93	0.43
1:C:167:GLY:HA3	1:C:213:SER:HB2	2.00	0.43
1:D:275:GLU:HB2	1:D:279:LYS:HD3	2.00	0.43
1:E:35:ARG:CD	3:E:4002:HOH:O	2.50	0.43
1:F:270:ARG:HH12	1:G:136:GLY:HA2	1.83	0.43
1:A:51:PHE:HB3	1:A:56:PHE:HB2	2.00	0.43
1:C:80:TYR:HA	1:C:251:GLY:HA2	2.00	0.43
1:E:188:LEU:O	1:E:190:PRO:HD3	2.17	0.43
1:E:80:TYR:HE1	1:E:253:MET:HB3	1.83	0.43
1:E:58:GLY:N	1:E:59:PRO:CD	2.81	0.43
1:F:50:ARG:O	1:F:54:LEU:CD1	2.66	0.43
1:G:262:GLU:CD	1:G:349:TYR:O	2.56	0.43
1:G:31:LEU:HB3	1:G:32:PRO:HD3	1.99	0.43
1:I:250:TRP:CE2	1:I:301:ALA:HB1	2.53	0.43
1:A:346:THR:CG2	3:D:3043:HOH:O	2.57	0.43
1:F:23:ARG:O	1:F:27:GLU:HB2	2.19	0.43
1:H:262:GLU:CD	1:H:349:TYR:O	2.56	0.43
1:A:346:THR:C	1:A:348:GLU:H	2.20	0.43
1:C:276:PRO:HD2	1:C:279:LYS:HB2	2.00	0.43
1:E:39:GLU:HG2	1:E:347:LEU:HD12	2.01	0.43
1:F:303:ARG:NH1	1:I:10:LEU:HD21	2.34	0.43
1:G:300:LEU:HD23	1:H:299:LEU:HD12	2.00	0.43
1:G:320:LEU:HD11	1:H:292:ALA:HB1	2.00	0.43
3:F:5031:HOH:O	1:G:346:THR:HG21	2.17	0.43
1:A:272:THR:CG2	1:A:273:PHE:HD1	2.31	0.43
1:A:82:LEU:HD11	1:A:93:VAL:HG21	2.00	0.43
1:D:103:PRO:HB3	1:D:240:CYS:SG	2.58	0.43
1:D:373:LEU:HB3	1:D:385:PHE:CZ	2.54	0.43
1:E:272:THR:O	1:E:274:GLY:N	2.39	0.43
1:G:202:LYS:C	1:G:203:ARG:HD2	2.38	0.43
1:I:140:PRO:CG	1:I:141:TYR:H	2.31	0.43
1:I:126:VAL:O	1:I:170:ALA:HA	2.18	0.43
1:I:334:ARG:HA	1:I:355:MET:HE2	1.99	0.43
1:I:373:LEU:HB3	1:I:385:PHE:CZ	2.53	0.43
1:A:272:THR:OG1	1:D:139:ASP:HB2	2.18	0.43
1:D:140:PRO:HG2	3:D:3026:HOH:O	2.18	0.43
1:D:197:GLN:HA	1:D:197:GLN:NE2	2.31	0.43
1:E:360:THR:HG21	2:E:4001:FAD:HM73	2.00	0.43
1:F:373:LEU:HD11	1:I:281:GLN:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:286:LYS:O	1:H:290:MET:HG3	2.19	0.43
1:H:383:ASN:C	1:H:383:ASN:HD22	2.22	0.43
1:I:234:LEU:HD22	1:I:238:LEU:CG	2.48	0.43
1:I:272:THR:C	1:I:274:GLY:N	2.71	0.43
1:I:78:ILE:HD12	1:I:82:LEU:HD12	2.01	0.43
1:D:127:GLY:HA2	1:D:172:LEU:O	2.18	0.43
1:D:41:GLY:HA2	1:D:208:ARG:HB3	1.99	0.43
1:E:280:LYS:HB2	1:E:283:VAL:HG22	1.99	0.43
1:E:58:GLY:N	1:E:101:MET:CE	2.81	0.43
1:F:262:GLU:CD	1:F:349:TYR:O	2.56	0.43
1:H:272:THR:HG21	2:I:8001:FAD:H61A	1.83	0.43
1:E:47:LEU:HD12	1:E:47:LEU:HA	1.75	0.43
1:G:130:GLY:HA2	1:G:164:ILE:HD12	2.01	0.43
1:G:197:GLN:HE21	1:G:197:GLN:CA	2.25	0.43
1:I:310:GLU:HG3	1:I:312:LYS:HE2	2.01	0.43
1:I:207:LEU:N	1:I:357:ASN:HD22	2.09	0.43
1:A:300:LEU:HD22	1:C:5:TYR:CE2	2.54	0.43
1:D:140:PRO:HD2	3:D:3026:HOH:O	2.18	0.43
1:D:23:ARG:O	1:D:27:GLU:HB2	2.19	0.43
1:F:136:GLY:HA2	1:G:270:ARG:HH12	1.84	0.43
1:G:278:ALA:CB	1:H:382:LEU:HD12	2.49	0.43
1:H:82:LEU:HD11	1:H:93:VAL:HG21	2.01	0.43
1:A:101:MET:HE2	1:A:120:LEU:C	2.38	0.43
1:A:281:GLN:HG3	3:A:1049:HOH:O	2.17	0.43
1:A:61:LEU:HA	1:A:62:PRO:HD3	1.86	0.43
1:C:323:ARG:NH1	1:C:324:GLN:OE1	2.51	0.43
1:C:373:LEU:HB3	1:C:385:PHE:CZ	2.54	0.43
1:H:260:TYR:HB2	1:H:290:MET:HE2	2.01	0.43
1:G:5:TYR:CE2	1:H:304:LEU:HD13	2.54	0.43
1:A:345:ILE:HB	1:D:206:SER:HB3	2.01	0.42
1:E:103:PRO:HB3	1:E:240:CYS:SG	2.58	0.42
1:G:292:ALA:CB	1:H:320:LEU:HD11	2.49	0.42
1:G:346:THR:HG22	1:G:348:GLU:CB	2.49	0.42
1:I:367:THR:OG1	1:I:370:VAL:HG13	2.19	0.42
1:F:342:GLY:O	1:F:345:ILE:HG12	2.19	0.42
1:G:364:TYR:C	1:G:364:TYR:HD1	2.23	0.42
1:H:237:PRO:O	1:H:240:CYS:HB2	2.19	0.42
1:I:163:TRP:O	2:I:8001:FAD:C4X	2.67	0.42
1:A:327:TRP:HA	1:A:327:TRP:CE3	2.54	0.42
1:A:34:ILE:HG12	1:A:86:ASP:HB2	2.01	0.42
1:D:133:GLU:OE2	1:D:161:LYS:NZ	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:ARG:HB3	1:E:277:LEU:HD22	2.02	0.42
1:E:56:PHE:O	1:E:59:PRO:HD3	2.18	0.42
1:H:126:VAL:O	1:H:170:ALA:HA	2.19	0.42
1:H:259:VAL:HG23	1:H:290:MET:CE	2.50	0.42
1:A:145:LYS:HA	1:A:147:ARG:HH12	1.84	0.42
1:A:31:LEU:N	1:A:32:PRO:CD	2.83	0.42
1:C:347:LEU:HG	1:E:205:MET:HG2	2.02	0.42
1:D:96:GLN:HG3	1:D:101:MET:HE3	2.00	0.42
1:E:158:ASN:OD1	1:E:219:GLU:N	2.43	0.42
1:G:62:PRO:HA	1:G:63:PRO:HD3	1.93	0.42
1:H:90:ARG:CZ	1:H:248:ILE:HG12	2.50	0.42
1:C:110:GLU:HG3	1:C:114:ARG:CZ	2.48	0.42
1:D:147:ARG:HG2	1:D:147:ARG:NH1	2.34	0.42
1:D:34:ILE:HG12	1:D:86:ASP:HB2	2.00	0.42
1:E:147:ARG:O	1:E:157:LEU:HA	2.19	0.42
1:E:260:TYR:O	1:E:264:VAL:HG13	2.19	0.42
1:E:126:VAL:HG13	1:E:169:LEU:O	2.20	0.42
1:E:236:ALA:HB3	1:E:237:PRO:CD	2.50	0.42
1:H:144:MET:SD	1:H:178:LYS:HG3	2.60	0.42
1:H:277:LEU:HA	1:H:277:LEU:HD12	1.75	0.42
1:I:25:PHE:CD2	1:I:54:LEU:HD22	2.55	0.42
1:C:241:LEU:O	1:C:245:ARG:HG3	2.19	0.42
1:C:367:THR:OG1	1:C:370:VAL:HG13	2.20	0.42
2:A:1001:FAD:N6A	1:D:280:LYS:HE2	2.35	0.42
1:D:337:ARG:O	1:D:337:ARG:HD2	2.19	0.42
1:H:260:TYR:HA	1:H:290:MET:CE	2.50	0.42
1:H:345:ILE:HB	1:I:206:SER:HB3	2.02	0.42
1:C:62:PRO:HA	1:C:63:PRO:HD3	1.91	0.42
1:D:133:GLU:CG	1:D:161:LYS:HD3	2.49	0.42
1:D:203:ARG:HA	1:D:203:ARG:HD3	1.88	0.42
1:D:379:ILE:HG23	1:E:260:TYR:OH	2.19	0.42
1:H:346:THR:HB	3:H:7057:HOH:O	2.19	0.42
1:E:196:PHE:HD1	1:E:217:LEU:CD2	2.33	0.42
1:F:117:LEU:HB2	1:F:118:PRO:HD3	2.02	0.42
1:F:276:PRO:HD2	1:F:279:LYS:CB	2.47	0.42
1:F:359:GLU:HG3	1:G:337:ARG:CZ	2.50	0.42
1:H:272:THR:C	1:H:274:GLY:H	2.23	0.42
1:I:140:PRO:CG	1:I:234:LEU:HD21	2.49	0.42
1:A:99:LEU:HB3	1:A:129:PHE:HB2	2.02	0.42
1:D:161:LYS:HB2	1:D:215:LEU:HB2	2.01	0.42
1:D:337:ARG:HB3	1:D:355:MET:HE1	1.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:VAL:CG1	1:E:169:LEU:O	2.68	0.42
1:H:146:THR:HG22	1:H:177:ALA:HB2	2.01	0.42
1:H:272:THR:HG21	2:I:8001:FAD:N7A	2.35	0.42
1:H:325:ASN:HD22	1:H:325:ASN:N	2.18	0.42
1:I:277:LEU:HD12	1:I:277:LEU:HA	1.78	0.42
1:I:47:LEU:HD12	1:I:47:LEU:HA	1.75	0.42
1:F:276:PRO:HG2	1:I:382:LEU:HD13	1.97	0.41
1:G:117:LEU:HB2	1:G:118:PRO:HD3	2.02	0.41
1:H:130:GLY:HA2	1:H:164:ILE:HD12	2.02	0.41
1:H:14:GLU:O	1:H:18:VAL:HG13	2.20	0.41
1:I:61:LEU:HA	1:I:62:PRO:HD3	1.86	0.41
1:A:126:VAL:O	1:A:170:ALA:HA	2.20	0.41
1:C:57:LEU:HB3	1:C:101:MET:CE	2.37	0.41
1:D:284:GLN:NE2	1:E:376:GLY:HA3	2.35	0.41
1:E:383:ASN:ND2	1:E:385:PHE:H	2.17	0.41
1:H:280:LYS:HE2	2:I:8001:FAD:N6A	2.35	0.41
1:I:110:GLU:CG	1:I:114:ARG:NH1	2.83	0.41
1:A:342:GLY:O	1:A:345:ILE:HG12	2.20	0.41
1:C:224:GLU:O	1:C:224:GLU:CG	2.61	0.41
1:C:264:VAL:HG23	1:C:268:LYS:HD2	2.01	0.41
1:D:107:TYR:HA	1:D:230:LYS:HB2	2.02	0.41
1:D:110:GLU:OE2	1:D:114:ARG:NH2	2.53	0.41
1:D:163:TRP:O	2:D:3001:FAD:C4X	2.68	0.41
1:D:172:LEU:HD12	1:D:172:LEU:HA	1.86	0.41
1:D:234:LEU:HD22	1:D:238:LEU:CG	2.50	0.41
1:E:20:LYS:HA	1:E:20:LYS:HE2	2.02	0.41
2:C:2001:FAD:H51A	1:E:277:LEU:HD21	2.01	0.41
1:E:377:ARG:HD2	3:E:4057:HOH:O	2.19	0.41
1:F:78:ILE:HD12	1:F:82:LEU:CD1	2.51	0.41
1:G:382:LEU:HB3	1:H:279:LYS:HG3	2.01	0.41
1:I:283:VAL:HG23	1:I:284:GLN:N	2.34	0.41
1:A:110:GLU:O	1:A:114:ARG:HG3	2.21	0.41
1:A:250:TRP:CE2	1:A:301:ALA:HB1	2.55	0.41
1:A:367:THR:O	1:A:370:VAL:HG22	2.20	0.41
1:C:242:THR:HG23	1:C:318:VAL:HG21	1.99	0.41
1:D:367:THR:OG1	1:D:370:VAL:HG13	2.20	0.41
1:E:270:ARG:HG2	1:E:270:ARG:NH1	2.34	0.41
1:F:162:MET:O	1:F:164:ILE:CD1	2.67	0.41
1:H:250:TRP:CE2	1:H:301:ALA:HB1	2.55	0.41
1:H:35:ARG:NH1	1:H:347:LEU:O	2.53	0.41
1:C:155:TRP:CD1	1:C:155:TRP:N	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:LYS:HB2	1:C:313:LEU:HD22	2.02	0.41
1:C:207:LEU:N	1:C:357:ASN:HD22	2.15	0.41
1:D:129:PHE:O	1:D:164:ILE:HG23	2.21	0.41
1:D:335:MET:O	1:D:339:ILE:HG13	2.20	0.41
1:D:35:ARG:CZ	1:D:35:ARG:HB2	2.50	0.41
1:D:207:LEU:HD22	1:D:360:THR:HG21	2.02	0.41
1:F:237:PRO:O	1:F:240:CYS:HB2	2.20	0.41
1:F:279:LYS:HG3	1:I:382:LEU:HB3	2.03	0.41
1:G:12:THR:HG1	1:G:15:GLU:HG3	1.83	0.41
1:H:56:PHE:O	1:H:59:PRO:HD3	2.21	0.41
1:C:250:TRP:CE2	1:C:301:ALA:HB1	2.55	0.41
1:D:228:LEU:HB3	1:D:231:ALA:CB	2.50	0.41
1:D:25:PHE:CD2	1:D:54:LEU:CD2	3.03	0.41
1:D:361:VAL:HA	1:D:364:TYR:CE1	2.56	0.41
1:E:234:LEU:HD22	1:E:238:LEU:CG	2.50	0.41
1:F:337:ARG:CG	1:F:355:MET:HE1	2.49	0.41
1:H:361:VAL:HA	1:H:364:TYR:CE1	2.56	0.41
1:I:264:VAL:HG12	1:I:287:LEU:HD22	2.03	0.41
1:D:126:VAL:HG12	1:D:171:HIS:HE1	1.84	0.41
1:D:273:PHE:N	1:D:273:PHE:CD1	2.89	0.41
1:D:383:ASN:HD22	1:D:383:ASN:C	2.24	0.41
1:F:172:LEU:HD11	1:F:188:LEU:CA	2.50	0.41
1:F:271:SER:CB	1:F:276:PRO:HA	2.50	0.41
1:G:47:LEU:HA	1:G:47:LEU:HD12	1.81	0.41
1:H:107:TYR:HA	1:H:230:LYS:HB2	2.02	0.41
1:H:80:TYR:HA	1:H:251:GLY:HA2	2.03	0.41
1:H:276:PRO:HD2	1:H:279:LYS:CB	2.50	0.41
1:I:12:THR:OG1	1:I:15:GLU:HG3	2.21	0.41
3:H:7042:HOH:O	1:I:203:ARG:NH1	2.45	0.41
3:H:7037:HOH:O	1:I:346:THR:CG2	2.62	0.41
1:I:361:VAL:HA	1:I:364:TYR:CE1	2.56	0.41
1:E:228:LEU:HA	1:E:229:PRO:HD2	1.90	0.41
1:E:325:ASN:N	1:E:325:ASN:HD22	2.19	0.41
1:F:197:GLN:HA	1:F:197:GLN:NE2	2.34	0.41
1:F:236:ALA:HB3	1:F:237:PRO:CD	2.50	0.41
1:I:207:LEU:HA	1:I:357:ASN:ND2	2.35	0.41
1:D:228:LEU:HB3	1:D:231:ALA:HB2	2.03	0.41
1:D:272:THR:C	1:D:274:GLY:N	2.74	0.41
1:F:360:THR:HG21	2:F:5001:FAD:HM73	2.03	0.41
1:G:226:LEU:HD12	1:G:226:LEU:HA	1.74	0.41
1:H:234:LEU:HD22	1:H:238:LEU:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:35:ARG:HH11	1:I:35:ARG:CG	2.33	0.41
1:H:203:ARG:NH2	1:I:39:GLU:CD	2.75	0.41
1:A:126:VAL:H	1:A:171:HIS:CE1	2.39	0.41
1:C:337:ARG:HB3	1:C:355:MET:CE	2.50	0.41
1:D:117:LEU:HB2	1:D:118:PRO:HD3	2.03	0.41
1:E:253:MET:HE3	1:E:256:LEU:HD13	2.03	0.41
1:F:364:TYR:C	1:F:364:TYR:CD1	2.95	0.41
1:G:114:ARG:HG2	1:G:114:ARG:HH21	1.85	0.41
1:H:126:VAL:H	1:H:171:HIS:CE1	2.39	0.41
1:A:7:LEU:HD11	1:A:299:LEU:HD21	2.02	0.41
1:A:320:LEU:HD11	1:C:292:ALA:CB	2.51	0.41
1:D:326:VAL:HG11	1:D:362:TYR:HA	2.03	0.41
1:D:57:LEU:HB3	1:D:101:MET:CE	2.50	0.41
1:G:362:TYR:CE1	1:G:368:HIS:HB2	2.56	0.41
1:H:138:SER:C	1:H:140:PRO:HD3	2.41	0.41
1:A:281:GLN:HE21	1:E:282:LEU:H	1.69	0.40
1:A:286:LYS:O	1:A:290:MET:HG3	2.20	0.40
1:A:362:TYR:CE1	1:A:368:HIS:HB2	2.56	0.40
1:F:36:ASP:O	1:F:40:GLU:CG	2.62	0.40
1:I:205:MET:O	1:I:356:LEU:HD13	2.20	0.40
1:I:273:PHE:N	1:I:273:PHE:CD1	2.88	0.40
1:I:364:TYR:C	1:I:364:TYR:CD1	2.94	0.40
1:A:190:PRO:O	1:A:193:THR:CG2	2.65	0.40
1:A:327:TRP:HA	1:A:327:TRP:HE3	1.86	0.40
1:A:34:ILE:HG23	1:A:35:ARG:N	2.36	0.40
1:A:364:TYR:CD1	1:A:364:TYR:C	2.95	0.40
1:A:7:LEU:HD11	1:A:299:LEU:CD2	2.51	0.40
1:C:150:ARG:HD3	1:C:155:TRP:NE1	2.36	0.40
1:E:337:ARG:CG	1:E:355:MET:HE3	2.50	0.40
1:F:146:THR:O	1:F:177:ALA:HB1	2.20	0.40
1:F:56:PHE:O	1:F:59:PRO:HD3	2.21	0.40
1:G:282:LEU:H	1:I:281:GLN:HE22	1.62	0.40
1:H:337:ARG:HB2	1:H:355:MET:HE2	2.04	0.40
1:C:293:TRP:CZ3	1:C:335:MET:HE1	2.56	0.40
1:D:205:MET:O	1:D:356:LEU:HD13	2.21	0.40
1:E:107:TYR:HA	1:E:230:LYS:HE3	2.02	0.40
1:H:140:PRO:O	1:H:144:MET:HB2	2.21	0.40
1:A:57:LEU:HB3	1:A:101:MET:HE3	2.02	0.40
1:A:228:LEU:HB3	1:A:231:ALA:CB	2.51	0.40
1:C:99:LEU:HB3	1:C:129:PHE:CG	2.56	0.40
1:C:107:TYR:HB3	1:C:231:ALA:N	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:PRO:O	1:D:193:THR:CG2	2.69	0.40
1:G:375:LEU:O	1:G:379:ILE:HG13	2.21	0.40
1:H:199:ARG:HH11	1:H:199:ARG:CG	2.34	0.40
1:I:383:ASN:ND2	1:I:385:PHE:H	2.20	0.40
1:C:270:ARG:O	1:C:271:SER:CB	2.68	0.40
1:D:114:ARG:HG2	1:D:114:ARG:HH21	1.86	0.40
1:D:48:ILE:CB	1:D:49:PRO:CD	2.99	0.40
1:E:234:LEU:O	1:E:238:LEU:HG	2.21	0.40
1:E:270:ARG:CG	1:E:270:ARG:HH11	2.35	0.40
1:F:10:LEU:N	1:F:10:LEU:HD23	2.36	0.40
1:F:230:LYS:C	1:F:232:LEU:HD13	2.40	0.40
1:G:103:PRO:HB3	1:G:240:CYS:SG	2.62	0.40
1:G:352:ILE:HG22	3:G:6071:HOH:O	2.21	0.40
1:H:203:ARG:NH2	1:I:39:GLU:CB	2.83	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:PRO:O	1:G:24:ARG:NH1[1_645]	2.10	0.10
1:I:64:GLU:OE1	3:E:4008:HOH:O[1_556]	2.18	0.02

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	374/385 (97%)	359 (96%)	14 (4%)	1 (0%)	41 45
1	C	374/385 (97%)	351 (94%)	19 (5%)	4 (1%)	14 11
1	D	374/385 (97%)	356 (95%)	16 (4%)	2 (0%)	29 30
1	E	374/385 (97%)	355 (95%)	19 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	374/385 (97%)	352 (94%)	21 (6%)	1 (0%)	41	45
1	G	374/385 (97%)	357 (96%)	13 (4%)	4 (1%)	14	11
1	H	374/385 (97%)	360 (96%)	14 (4%)	0	100	100
1	I	374/385 (97%)	360 (96%)	12 (3%)	2 (0%)	29	30
All	All	2992/3080 (97%)	2850 (95%)	128 (4%)	14 (0%)	29	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	188	LEU
1	C	275	GLU
1	D	275	GLU
1	D	276	PRO
1	G	275	GLU
1	C	273	PHE
1	F	231	ALA
1	I	273	PHE
1	C	276	PRO
1	G	273	PHE
1	G	276	PRO
1	A	35	ARG
1	I	276	PRO
1	G	123	GLY

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	308/310 (99%)	280 (91%)	28 (9%)	9	8
1	C	308/310 (99%)	282 (92%)	26 (8%)	11	10
1	D	308/310 (99%)	283 (92%)	25 (8%)	11	11
1	E	308/310 (99%)	277 (90%)	31 (10%)	7	6
1	F	308/310 (99%)	278 (90%)	30 (10%)	8	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	308/310 (99%)	274 (89%)	34 (11%)	6	5
1	H	308/310 (99%)	281 (91%)	27 (9%)	10	9
1	I	308/310 (99%)	286 (93%)	22 (7%)	14	15
All	All	2464/2480 (99%)	2241 (91%)	223 (9%)	9	8

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	19	GLN
1	A	28	LYS
1	A	31	LEU
1	A	35	ARG
1	A	47	LEU
1	A	78	ILE
1	A	83	GLU
1	A	126	VAL
1	A	145	LYS
1	A	162	MET
1	A	193	THR
1	A	197	GLN
1	A	205	MET
1	A	226	LEU
1	A	228	LEU
1	A	230	LYS
1	A	232	LEU
1	A	234	LEU
1	A	264	VAL
1	A	270	ARG
1	A	272	THR
1	A	277	LEU
1	A	283	VAL
1	A	364	TYR
1	A	373	LEU
1	A	378	GLU
1	A	383	ASN
1	C	17	GLU
1	C	19	GLN
1	C	27	GLU
1	C	40	GLU
1	C	47	LEU

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Mol	Chain	Res	Type
1	C	53	GLU
1	C	78	ILE
1	C	83	GLU
1	C	150	ARG
1	C	153	ASP
1	C	162	MET
1	C	193	THR
1	C	197	GLN
1	C	205	MET
1	C	222	VAL
1	C	226	LEU
1	C	228	LEU
1	C	230	LYS
1	C	234	LEU
1	C	264	VAL
1	C	270	ARG
1	C	277	LEU
1	C	364	TYR
1	C	373	LEU
1	C	378	GLU
1	C	383	ASN
1	D	17	GLU
1	D	19	GLN
1	D	27	GLU
1	D	28	LYS
1	D	40	GLU
1	D	78	ILE
1	D	126	VAL
1	D	153	ASP
1	D	156	VAL
1	D	162	MET
1	D	193	THR
1	D	203	ARG
1	D	226	LEU
1	D	228	LEU
1	D	230	LYS
1	D	234	LEU
1	D	264	VAL
1	D	268	LYS
1	D	270	ARG
1	D	277	LEU
1	D	337	ARG

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Mol	Chain	Res	Type
1	D	364	TYR
1	D	373	LEU
1	D	378	GLU
1	D	383	ASN
1	E	17	GLU
1	E	19	GLN
1	E	25	PHE
1	E	27	GLU
1	E	28	LYS
1	E	35	ARG
1	E	40	GLU
1	E	47	LEU
1	E	78	ILE
1	E	83	GLU
1	E	126	VAL
1	E	156	VAL
1	E	162	MET
1	E	174	VAL
1	E	193	THR
1	E	199	ARG
1	E	202	LYS
1	E	226	LEU
1	E	228	LEU
1	E	230	LYS
1	E	232	LEU
1	E	234	LEU
1	E	264	VAL
1	E	270	ARG
1	E	271	SER
1	E	277	LEU
1	E	323	ARG
1	E	364	TYR
1	E	373	LEU
1	E	378	GLU
1	E	383	ASN
1	F	1	MET
1	F	10	LEU
1	F	17	GLU
1	F	19	GLN
1	F	27	GLU
1	F	35	ARG
1	F	40	GLU

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Mol	Chain	Res	Type
1	F	47	LEU
1	F	78	ILE
1	F	83	GLU
1	F	126	VAL
1	F	149	ARG
1	F	150	ARG
1	F	162	MET
1	F	193	THR
1	F	203	ARG
1	F	226	LEU
1	F	228	LEU
1	F	230	LYS
1	F	234	LEU
1	F	253	MET
1	F	264	VAL
1	F	270	ARG
1	F	272	THR
1	F	277	LEU
1	F	320	LEU
1	F	364	TYR
1	F	373	LEU
1	F	378	GLU
1	F	383	ASN
1	G	7	LEU
1	G	8	GLU
1	G	14	GLU
1	G	17	GLU
1	G	19	GLN
1	G	27	GLU
1	G	28	LYS
1	G	35	ARG
1	G	47	LEU
1	G	64	GLU
1	G	78	ILE
1	G	83	GLU
1	G	115	GLU
1	G	125	MET
1	G	126	VAL
1	G	150	ARG
1	G	156	VAL
1	G	193	THR
1	G	197	GLN

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Mol	Chain	Res	Type
1	G	203	ARG
1	G	226	LEU
1	G	228	LEU
1	G	230	LYS
1	G	234	LEU
1	G	264	VAL
1	G	270	ARG
1	G	271	SER
1	G	275	GLU
1	G	277	LEU
1	G	337	ARG
1	G	364	TYR
1	G	373	LEU
1	G	378	GLU
1	G	383	ASN
1	H	17	GLU
1	H	19	GLN
1	H	27	GLU
1	H	47	LEU
1	H	57	LEU
1	H	78	ILE
1	H	83	GLU
1	H	126	VAL
1	H	162	MET
1	H	193	THR
1	H	197	GLN
1	H	226	LEU
1	H	228	LEU
1	H	230	LYS
1	H	232	LEU
1	H	234	LEU
1	H	264	VAL
1	H	268	LYS
1	H	270	ARG
1	H	271	SER
1	H	272	THR
1	H	277	LEU
1	H	337	ARG
1	H	364	TYR
1	H	373	LEU
1	H	378	GLU
1	H	383	ASN

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Mol	Chain	Res	Type
1	I	17	GLU
1	I	19	GLN
1	I	27	GLU
1	I	40	GLU
1	I	47	LEU
1	I	78	ILE
1	I	126	VAL
1	I	140	PRO
1	I	193	THR
1	I	197	GLN
1	I	226	LEU
1	I	228	LEU
1	I	230	LYS
1	I	232	LEU
1	I	234	LEU
1	I	264	VAL
1	I	270	ARG
1	I	277	LEU
1	I	364	TYR
1	I	373	LEU
1	I	378	GLU
1	I	383	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	197	GLN
1	A	281	GLN
1	A	284	GLN
1	A	325	ASN
1	A	357	ASN
1	A	368	HIS
1	A	383	ASN
1	C	19	GLN
1	C	46	HIS
1	C	197	GLN
1	C	281	GLN
1	C	284	GLN
1	C	325	ASN
1	C	357	ASN
1	C	368	HIS

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Mol	Chain	Res	Type
1	C	383	ASN
1	D	171	HIS
1	D	197	GLN
1	D	281	GLN
1	D	284	GLN
1	D	325	ASN
1	D	357	ASN
1	D	383	ASN
1	E	19	GLN
1	E	166	ASN
1	E	197	GLN
1	E	281	GLN
1	E	284	GLN
1	E	325	ASN
1	E	357	ASN
1	E	368	HIS
1	E	383	ASN
1	F	19	GLN
1	F	197	GLN
1	F	281	GLN
1	F	284	GLN
1	F	325	ASN
1	F	357	ASN
1	F	368	HIS
1	F	383	ASN
1	G	19	GLN
1	G	197	GLN
1	G	281	GLN
1	G	284	GLN
1	G	325	ASN
1	G	357	ASN
1	G	383	ASN
1	H	19	GLN
1	H	197	GLN
1	H	281	GLN
1	H	284	GLN
1	H	325	ASN
1	H	357	ASN
1	H	383	ASN
1	I	19	GLN
1	I	197	GLN
1	I	281	GLN

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Mol	Chain	Res	Type
1	I	284	GLN
1	I	325	ASN
1	I	357	ASN
1	I	368	HIS
1	I	383	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 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	3001	-	51,58,58	2.00	13 (25%)	60,89,89	2.21	17 (28%)
2	FAD	F	5001	-	51,58,58	2.08	11 (21%)	60,89,89	2.27	16 (26%)
2	FAD	G	6001	-	51,58,58	2.05	12 (23%)	60,89,89	2.23	16 (26%)
2	FAD	I	8001	-	51,58,58	2.02	15 (29%)	60,89,89	2.20	17 (28%)
2	FAD	H	7001	-	51,58,58	2.03	13 (25%)	60,89,89	2.23	17 (28%)
2	FAD	A	1001	-	51,58,58	2.07	12 (23%)	60,89,89	2.22	15 (25%)
2	FAD	C	2001	-	51,58,58	2.07	13 (25%)	60,89,89	2.25	16 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	E	4001	-	51,58,58	2.08	13 (25%)	60,89,89	2.24	15 (25%)

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	3001	-	-	9/30/50/50	0/6/6/6
2	FAD	F	5001	-	-	7/30/50/50	0/6/6/6
2	FAD	G	6001	-	-	11/30/50/50	0/6/6/6
2	FAD	I	8001	-	-	11/30/50/50	0/6/6/6
2	FAD	H	7001	-	-	6/30/50/50	0/6/6/6
2	FAD	A	1001	-	-	4/30/50/50	0/6/6/6
2	FAD	C	2001	-	-	6/30/50/50	0/6/6/6
2	FAD	E	4001	-	-	8/30/50/50	0/6/6/6

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	FAD	O4B-C1B	-6.76	1.31	1.41
2	I	8001	FAD	O4B-C4B	6.59	1.59	1.45
2	G	6001	FAD	O4B-C4B	6.56	1.59	1.45
2	D	3001	FAD	O4B-C4B	6.54	1.59	1.45
2	C	2001	FAD	O4B-C4B	6.52	1.59	1.45
2	H	7001	FAD	O4B-C4B	6.49	1.59	1.45
2	A	1001	FAD	O4B-C4B	6.45	1.59	1.45
2	E	4001	FAD	O4B-C4B	6.40	1.59	1.45
2	G	6001	FAD	O4B-C1B	-6.40	1.32	1.41
2	F	5001	FAD	O4B-C4B	6.39	1.59	1.45
2	E	4001	FAD	O4B-C1B	-6.37	1.32	1.41
2	C	2001	FAD	O4B-C1B	-6.21	1.32	1.41
2	F	5001	FAD	O4B-C1B	-6.17	1.32	1.41
2	H	7001	FAD	O4B-C1B	-6.04	1.32	1.41
2	I	8001	FAD	O4B-C1B	-5.12	1.33	1.41
2	F	5001	FAD	C4X-C10	4.87	1.43	1.38
2	I	8001	FAD	C4X-C10	4.58	1.43	1.38
2	D	3001	FAD	O4B-C1B	-4.48	1.34	1.41
2	E	4001	FAD	C4X-C10	4.41	1.43	1.38
2	C	2001	FAD	C10-N1	4.39	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5001	FAD	C10-N1	4.36	1.38	1.33
2	E	4001	FAD	C10-N1	4.25	1.38	1.33
2	H	7001	FAD	C10-N1	4.20	1.38	1.33
2	G	6001	FAD	C4X-C10	4.14	1.43	1.38
2	D	3001	FAD	C4X-C10	4.13	1.43	1.38
2	I	8001	FAD	C10-N1	4.12	1.38	1.33
2	I	8001	FAD	C4X-N5	4.02	1.39	1.33
2	A	1001	FAD	C4X-C10	4.02	1.42	1.38
2	D	3001	FAD	C10-N1	4.01	1.38	1.33
2	C	2001	FAD	C4X-C10	3.98	1.42	1.38
2	C	2001	FAD	C4X-N5	3.96	1.39	1.33
2	G	6001	FAD	C10-N1	3.96	1.38	1.33
2	F	5001	FAD	C4X-N5	3.96	1.39	1.33
2	A	1001	FAD	C10-N1	3.91	1.38	1.33
2	H	7001	FAD	C4X-C10	3.87	1.42	1.38
2	D	3001	FAD	C4X-N5	3.82	1.38	1.33
2	A	1001	FAD	C3B-C4B	3.82	1.62	1.53
2	D	3001	FAD	C3B-C4B	3.82	1.62	1.53
2	C	2001	FAD	C3B-C4B	3.78	1.62	1.53
2	I	8001	FAD	C3B-C4B	3.78	1.62	1.53
2	G	6001	FAD	C4X-N5	3.76	1.38	1.33
2	G	6001	FAD	C3B-C4B	3.76	1.62	1.53
2	E	4001	FAD	C3B-C4B	3.70	1.62	1.53
2	F	5001	FAD	C3B-C4B	3.67	1.62	1.53
2	H	7001	FAD	C3B-C4B	3.66	1.62	1.53
2	E	4001	FAD	C4X-N5	3.61	1.38	1.33
2	H	7001	FAD	C4X-N5	3.60	1.38	1.33
2	A	1001	FAD	C4X-N5	3.56	1.38	1.33
2	A	1001	FAD	C2A-N3A	3.51	1.37	1.32
2	D	3001	FAD	C4A-N3A	3.38	1.40	1.35
2	F	5001	FAD	C4-N3	3.37	1.38	1.33
2	E	4001	FAD	C4-N3	3.28	1.38	1.33
2	H	7001	FAD	O5B-C5B	-3.09	1.32	1.44
2	C	2001	FAD	O5B-C5B	-3.01	1.33	1.44
2	E	4001	FAD	O5B-C5B	-3.00	1.33	1.44
2	E	4001	FAD	C4A-N3A	2.94	1.39	1.35
2	A	1001	FAD	O5B-C5B	-2.93	1.33	1.44
2	F	5001	FAD	O5B-C5B	-2.93	1.33	1.44
2	I	8001	FAD	O5B-C5B	-2.91	1.33	1.44
2	G	6001	FAD	O5B-C5B	-2.91	1.33	1.44
2	G	6001	FAD	C2A-N3A	2.89	1.36	1.32
2	G	6001	FAD	C4-N3	2.86	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	7001	FAD	C4-N3	2.84	1.38	1.33
2	C	2001	FAD	C4-N3	2.83	1.38	1.33
2	D	3001	FAD	O5B-C5B	-2.82	1.33	1.44
2	D	3001	FAD	C2A-N1A	2.82	1.39	1.33
2	A	1001	FAD	C4-N3	2.80	1.37	1.33
2	C	2001	FAD	C2A-N3A	2.80	1.36	1.32
2	C	2001	FAD	C4A-N3A	2.67	1.39	1.35
2	D	3001	FAD	O2B-C2B	-2.60	1.36	1.43
2	C	2001	FAD	C2B-C1B	-2.57	1.49	1.53
2	H	7001	FAD	C4A-N3A	2.57	1.39	1.35
2	D	3001	FAD	C4-N3	2.53	1.37	1.33
2	F	5001	FAD	C2B-C1B	-2.52	1.49	1.53
2	D	3001	FAD	C2B-C1B	-2.50	1.50	1.53
2	I	8001	FAD	O2B-C2B	-2.47	1.37	1.43
2	I	8001	FAD	C4-N3	2.40	1.37	1.33
2	H	7001	FAD	C2B-C1B	-2.39	1.50	1.53
2	E	4001	FAD	C2A-N3A	2.39	1.35	1.32
2	I	8001	FAD	C4A-N3A	2.37	1.38	1.35
2	F	5001	FAD	C2A-N3A	2.36	1.35	1.32
2	A	1001	FAD	C4A-N3A	2.34	1.38	1.35
2	H	7001	FAD	C2A-N1A	2.30	1.38	1.33
2	E	4001	FAD	C2A-N1A	2.29	1.38	1.33
2	G	6001	FAD	C4A-N3A	2.29	1.38	1.35
2	A	1001	FAD	C9A-N10	2.26	1.41	1.38
2	I	8001	FAD	C5X-N5	2.25	1.39	1.35
2	H	7001	FAD	C2A-N3A	2.25	1.35	1.32
2	I	8001	FAD	C2A-N3A	2.25	1.35	1.32
2	I	8001	FAD	C2A-N1A	2.15	1.37	1.33
2	E	4001	FAD	C6-C7	2.12	1.43	1.37
2	F	5001	FAD	C9A-N10	2.12	1.41	1.38
2	G	6001	FAD	C5X-N5	2.11	1.38	1.35
2	G	6001	FAD	C2B-C1B	-2.10	1.50	1.53
2	C	2001	FAD	C9A-N10	2.10	1.41	1.38
2	I	8001	FAD	C9A-N10	2.09	1.41	1.38
2	A	1001	FAD	O2B-C2B	-2.07	1.38	1.43
2	D	3001	FAD	C5X-N5	2.04	1.38	1.35
2	I	8001	FAD	C2B-C1B	-2.03	1.50	1.53
2	E	4001	FAD	O2B-C2B	-2.01	1.38	1.43
2	C	2001	FAD	C5X-N5	2.00	1.38	1.35
2	H	7001	FAD	C9A-N10	2.00	1.41	1.38

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	6001	FAD	O4B-C4B-C3B	-7.34	90.59	105.11
2	F	5001	FAD	C4-N3-C2	7.30	121.31	115.14
2	C	2001	FAD	O4B-C4B-C3B	-7.29	90.68	105.11
2	E	4001	FAD	O4B-C4B-C3B	-7.29	90.70	105.11
2	F	5001	FAD	O4B-C4B-C3B	-7.28	90.71	105.11
2	A	1001	FAD	O4B-C4B-C3B	-7.28	90.71	105.11
2	H	7001	FAD	O4B-C4B-C3B	-7.12	91.02	105.11
2	C	2001	FAD	C4-N3-C2	7.08	121.12	115.14
2	I	8001	FAD	O4B-C4B-C3B	-7.07	91.13	105.11
2	H	7001	FAD	C4-N3-C2	6.99	121.04	115.14
2	D	3001	FAD	O4B-C4B-C3B	-6.91	91.45	105.11
2	D	3001	FAD	C4-N3-C2	6.89	120.96	115.14
2	E	4001	FAD	C4-N3-C2	6.89	120.96	115.14
2	G	6001	FAD	C4-N3-C2	6.74	120.83	115.14
2	A	1001	FAD	C4-N3-C2	6.67	120.77	115.14
2	I	8001	FAD	C4-N3-C2	6.63	120.74	115.14
2	E	4001	FAD	N3A-C2A-N1A	-5.22	120.52	128.68
2	A	1001	FAD	N3A-C2A-N1A	-5.06	120.77	128.68
2	F	5001	FAD	N3A-C2A-N1A	-5.02	120.83	128.68
2	C	2001	FAD	N3A-C2A-N1A	-4.97	120.91	128.68
2	H	7001	FAD	N3A-C2A-N1A	-4.94	120.96	128.68
2	G	6001	FAD	N3A-C2A-N1A	-4.89	121.03	128.68
2	I	8001	FAD	N3A-C2A-N1A	-4.84	121.11	128.68
2	H	7001	FAD	C1'-N10-C9A	4.71	122.00	118.29
2	D	3001	FAD	N3A-C2A-N1A	-4.70	121.33	128.68
2	A	1001	FAD	C4X-N5-C5X	4.68	121.45	116.77
2	I	8001	FAD	C2B-C3B-C4B	4.65	111.68	102.64
2	A	1001	FAD	C1'-N10-C9A	4.64	121.94	118.29
2	G	6001	FAD	C2B-C3B-C4B	4.62	111.62	102.64
2	E	4001	FAD	C2B-C3B-C4B	4.61	111.59	102.64
2	F	5001	FAD	C2B-C3B-C4B	4.60	111.59	102.64
2	E	4001	FAD	C1'-N10-C9A	4.60	121.91	118.29
2	D	3001	FAD	C2B-C3B-C4B	4.58	111.54	102.64
2	A	1001	FAD	C2B-C3B-C4B	4.58	111.54	102.64
2	I	8001	FAD	C1'-N10-C9A	4.56	121.88	118.29
2	C	2001	FAD	C2B-C3B-C4B	4.55	111.48	102.64
2	F	5001	FAD	C1'-N10-C9A	4.54	121.87	118.29
2	I	8001	FAD	C4X-N5-C5X	4.53	121.30	116.77
2	H	7001	FAD	C2B-C3B-C4B	4.50	111.38	102.64
2	C	2001	FAD	C4X-N5-C5X	4.49	121.26	116.77
2	D	3001	FAD	C4X-N5-C5X	4.47	121.24	116.77
2	G	6001	FAD	C1'-N10-C9A	4.46	121.81	118.29
2	G	6001	FAD	C4X-N5-C5X	4.46	121.23	116.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	5001	FAD	C4X-N5-C5X	4.41	121.17	116.77
2	H	7001	FAD	C4X-N5-C5X	4.39	121.16	116.77
2	C	2001	FAD	C1'-N10-C9A	4.32	121.70	118.29
2	E	4001	FAD	C4X-N5-C5X	4.28	121.05	116.77
2	D	3001	FAD	C1'-N10-C9A	4.08	121.50	118.29
2	C	2001	FAD	O3B-C3B-C2B	-3.86	99.32	111.82
2	A	1001	FAD	O3B-C3B-C2B	-3.85	99.37	111.82
2	H	7001	FAD	O3B-C3B-C2B	-3.85	99.38	111.82
2	D	3001	FAD	O3B-C3B-C2B	-3.84	99.38	111.82
2	E	4001	FAD	O3B-C3B-C2B	-3.81	99.48	111.82
2	G	6001	FAD	O3B-C3B-C2B	-3.81	99.49	111.82
2	I	8001	FAD	O3B-C3B-C2B	-3.80	99.54	111.82
2	F	5001	FAD	O3B-C3B-C2B	-3.79	99.57	111.82
2	D	3001	FAD	C4A-C5A-N7A	-3.77	105.47	109.40
2	I	8001	FAD	C4-C4X-N5	3.02	122.05	118.60
2	G	6001	FAD	C4-C4X-N5	2.98	122.01	118.60
2	F	5001	FAD	C1B-N9A-C4A	-2.83	121.67	126.64
2	D	3001	FAD	C4-C4X-N5	2.81	121.81	118.60
2	A	1001	FAD	O5B-C5B-C4B	2.80	118.63	108.99
2	E	4001	FAD	C1B-N9A-C4A	-2.80	121.72	126.64
2	F	5001	FAD	C4X-C4-N3	-2.80	119.61	123.43
2	I	8001	FAD	C4A-C5A-N7A	-2.79	106.49	109.40
2	H	7001	FAD	O5B-C5B-C4B	2.79	118.59	108.99
2	I	8001	FAD	O5B-C5B-C4B	2.77	118.51	108.99
2	C	2001	FAD	O5B-C5B-C4B	2.76	118.51	108.99
2	C	2001	FAD	C4-C4X-N5	2.76	121.75	118.60
2	D	3001	FAD	O5B-C5B-C4B	2.76	118.49	108.99
2	G	6001	FAD	O5B-C5B-C4B	2.75	118.47	108.99
2	G	6001	FAD	C4A-C5A-N7A	-2.70	106.58	109.40
2	C	2001	FAD	C1B-N9A-C4A	-2.69	121.91	126.64
2	F	5001	FAD	C4-C4X-N5	2.66	121.63	118.60
2	F	5001	FAD	O5B-C5B-C4B	2.65	118.12	108.99
2	E	4001	FAD	C4-C4X-N5	2.64	121.61	118.60
2	E	4001	FAD	O5B-C5B-C4B	2.63	118.04	108.99
2	H	7001	FAD	C1B-N9A-C4A	-2.61	122.05	126.64
2	G	6001	FAD	C1B-N9A-C4A	-2.61	122.06	126.64
2	I	8001	FAD	C10-C4X-N5	-2.60	119.46	121.26
2	H	7001	FAD	C4-C4X-N5	2.59	121.56	118.60
2	A	1001	FAD	C4A-C5A-N7A	-2.59	106.70	109.40
2	G	6001	FAD	C4X-C4-N3	-2.56	119.93	123.43
2	C	2001	FAD	C4A-C5A-N7A	-2.56	106.73	109.40
2	G	6001	FAD	C10-C4X-N5	-2.55	119.50	121.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	FAD	C4X-C4-N3	-2.54	119.96	123.43
2	A	1001	FAD	C1B-N9A-C4A	-2.53	122.20	126.64
2	E	4001	FAD	C4A-C5A-N7A	-2.52	106.78	109.40
2	A	1001	FAD	C4X-C4-N3	-2.51	120.00	123.43
2	E	4001	FAD	C4X-C4-N3	-2.51	120.00	123.43
2	D	3001	FAD	C10-C4X-N5	-2.46	119.56	121.26
2	D	3001	FAD	C4X-C4-N3	-2.46	120.07	123.43
2	G	6001	FAD	O3B-C3B-C4B	-2.45	103.97	111.05
2	C	2001	FAD	O3B-C3B-C4B	-2.44	104.00	111.05
2	I	8001	FAD	O3B-C3B-C4B	-2.43	104.03	111.05
2	A	1001	FAD	O3B-C3B-C4B	-2.40	104.10	111.05
2	H	7001	FAD	C4A-C5A-N7A	-2.40	106.89	109.40
2	E	4001	FAD	O3B-C3B-C4B	-2.38	104.16	111.05
2	H	7001	FAD	O3B-C3B-C4B	-2.37	104.18	111.05
2	D	3001	FAD	O3B-C3B-C4B	-2.37	104.20	111.05
2	I	8001	FAD	C4X-C4-N3	-2.36	120.20	123.43
2	H	7001	FAD	C4X-C4-N3	-2.36	120.20	123.43
2	F	5001	FAD	O3B-C3B-C4B	-2.35	104.26	111.05
2	D	3001	FAD	C5B-C4B-C3B	-2.34	106.40	115.18
2	C	2001	FAD	C5B-C4B-C3B	-2.34	106.42	115.18
2	I	8001	FAD	C5B-C4B-C3B	-2.32	106.47	115.18
2	F	5001	FAD	C4A-C5A-N7A	-2.31	106.99	109.40
2	A	1001	FAD	C4-C4X-N5	2.30	121.23	118.60
2	G	6001	FAD	C5B-C4B-C3B	-2.30	106.57	115.18
2	A	1001	FAD	C5B-C4B-C3B	-2.29	106.59	115.18
2	H	7001	FAD	C5B-C4B-C3B	-2.28	106.64	115.18
2	E	4001	FAD	C5B-C4B-C3B	-2.27	106.66	115.18
2	F	5001	FAD	C5B-C4B-C3B	-2.26	106.72	115.18
2	E	4001	FAD	C4-C4X-C10	-2.24	118.47	119.95
2	C	2001	FAD	C10-C4X-N5	-2.24	119.71	121.26
2	D	3001	FAD	C1B-N9A-C4A	-2.23	122.72	126.64
2	F	5001	FAD	C4-C4X-C10	-2.22	118.48	119.95
2	G	6001	FAD	C4-C4X-C10	-2.21	118.49	119.95
2	I	8001	FAD	C4-C4X-C10	-2.20	118.50	119.95
2	F	5001	FAD	O2'-C2'-C3'	2.19	114.42	109.10
2	C	2001	FAD	C4-C4X-C10	-2.15	118.53	119.95
2	H	7001	FAD	O2'-C2'-C3'	2.10	114.20	109.10
2	A	1001	FAD	C10-C4X-N5	-2.08	119.82	121.26
2	H	7001	FAD	C4-C4X-C10	-2.06	118.59	119.95
2	I	8001	FAD	O2A-PA-O1A	2.04	122.31	112.24
2	D	3001	FAD	O2'-C2'-C3'	2.04	114.05	109.10
2	I	8001	FAD	C1B-N9A-C4A	-2.03	123.07	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	7001	FAD	C10-C4X-N5	-2.03	119.85	121.26
2	D	3001	FAD	C4-C4X-C10	-2.00	118.62	119.95

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	3001	FAD	C1'-C2'-C3'-O3'
2	D	3001	FAD	C1'-C2'-C3'-C4'
2	G	6001	FAD	C1'-C2'-C3'-C4'
2	G	6001	FAD	C5'-O5'-P-O1P
2	I	8001	FAD	C5'-O5'-P-O1P
2	H	7001	FAD	C1'-C2'-C3'-O3'
2	H	7001	FAD	C1'-C2'-C3'-C4'
2	A	1001	FAD	C1'-C2'-C3'-O3'
2	C	2001	FAD	C1'-C2'-C3'-O3'
2	C	2001	FAD	C1'-C2'-C3'-C4'
2	C	2001	FAD	O2'-C2'-C3'-C4'
2	D	3001	FAD	O2'-C2'-C3'-C4'
2	G	6001	FAD	O2'-C2'-C3'-C4'
2	H	7001	FAD	O2'-C2'-C3'-C4'
2	A	1001	FAD	O2'-C2'-C3'-C4'
2	E	4001	FAD	O2'-C2'-C3'-C4'
2	C	2001	FAD	O2'-C2'-C3'-O3'
2	H	7001	FAD	O2'-C2'-C3'-O3'
2	D	3001	FAD	C2'-C3'-C4'-O4'
2	F	5001	FAD	O2'-C2'-C3'-C4'
2	F	5001	FAD	C1'-C2'-C3'-O3'
2	G	6001	FAD	C1'-C2'-C3'-O3'
2	I	8001	FAD	C1'-C2'-C3'-O3'
2	E	4001	FAD	C1'-C2'-C3'-O3'
2	D	3001	FAD	O3'-C3'-C4'-O4'
2	I	8001	FAD	O2'-C2'-C3'-C4'
2	I	8001	FAD	O3'-C3'-C4'-O4'
2	A	1001	FAD	O2'-C2'-C3'-O3'
2	E	4001	FAD	O2'-C2'-C3'-O3'
2	I	8001	FAD	C2'-C3'-C4'-O4'
2	D	3001	FAD	O3'-C3'-C4'-C5'
2	D	3001	FAD	O2'-C2'-C3'-O3'
2	I	8001	FAD	O3'-C3'-C4'-C5'
2	F	5001	FAD	O2'-C2'-C3'-O3'
2	G	6001	FAD	O2'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
2	E	4001	FAD	O3'-C3'-C4'-O4'
2	D	3001	FAD	O4'-C4'-C5'-O5'
2	G	6001	FAD	O4'-C4'-C5'-O5'
2	F	5001	FAD	C5'-O5'-P-O3P
2	G	6001	FAD	C5'-O5'-P-O3P
2	I	8001	FAD	C5'-O5'-P-O3P
2	G	6001	FAD	O3'-C3'-C4'-C5'
2	E	4001	FAD	O3'-C3'-C4'-C5'
2	D	3001	FAD	P-O3P-PA-O1A
2	F	5001	FAD	P-O3P-PA-O1A
2	G	6001	FAD	P-O3P-PA-O2A
2	I	8001	FAD	P-O3P-PA-O1A
2	H	7001	FAD	P-O3P-PA-O1A
2	A	1001	FAD	P-O3P-PA-O1A
2	C	2001	FAD	P-O3P-PA-O1A
2	E	4001	FAD	P-O3P-PA-O1A
2	G	6001	FAD	O3'-C3'-C4'-O4'
2	I	8001	FAD	O2'-C2'-C3'-O3'
2	E	4001	FAD	C2'-C3'-C4'-O4'
2	G	6001	FAD	C5'-O5'-P-O2P
2	I	8001	FAD	C5'-O5'-P-O2P
2	F	5001	FAD	O3'-C3'-C4'-C5'
2	F	5001	FAD	O3'-C3'-C4'-O4'
2	I	8001	FAD	O4'-C4'-C5'-O5'
2	H	7001	FAD	O4'-C4'-C5'-O5'
2	C	2001	FAD	O4'-C4'-C5'-O5'
2	E	4001	FAD	O4'-C4'-C5'-O5'

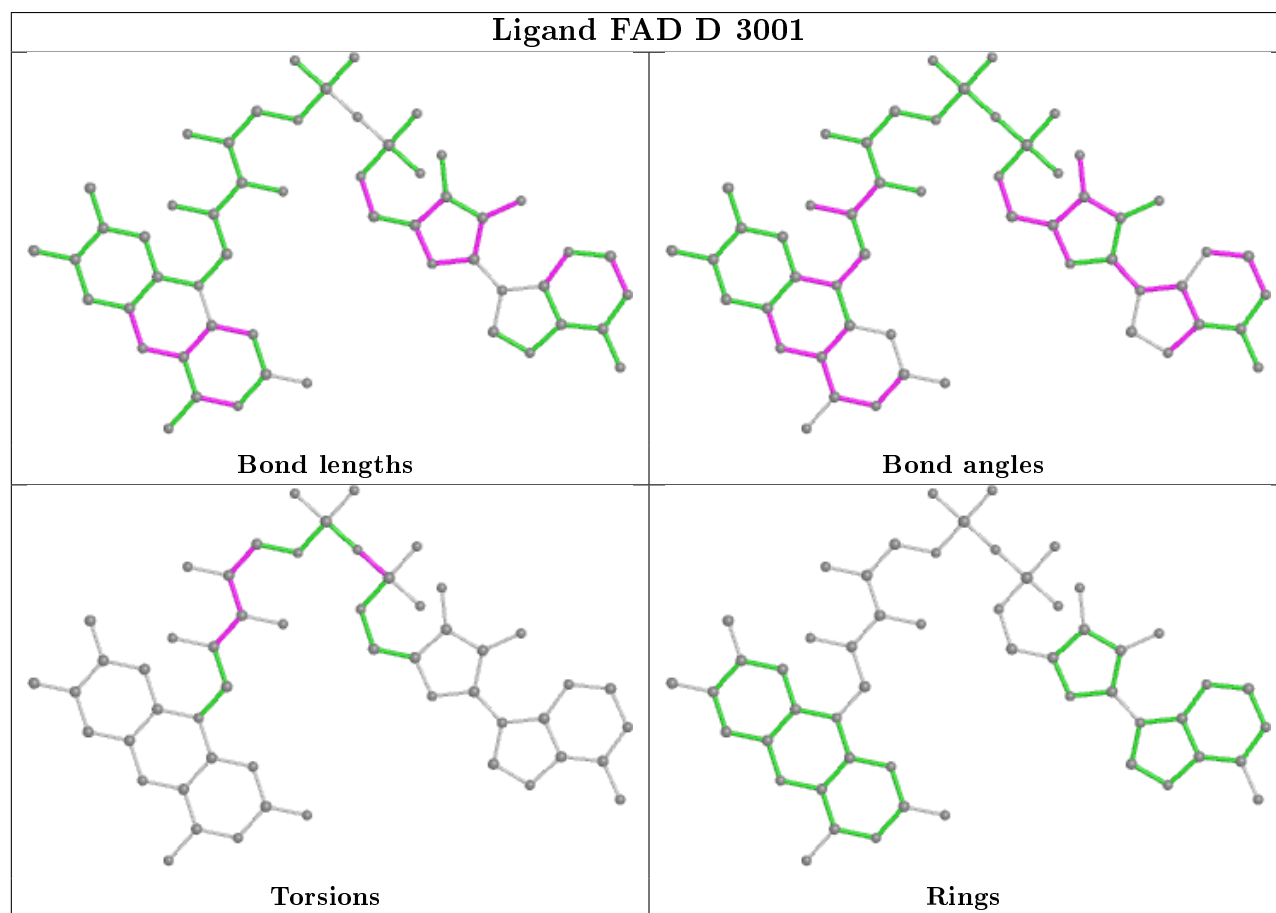
There are no ring outliers.

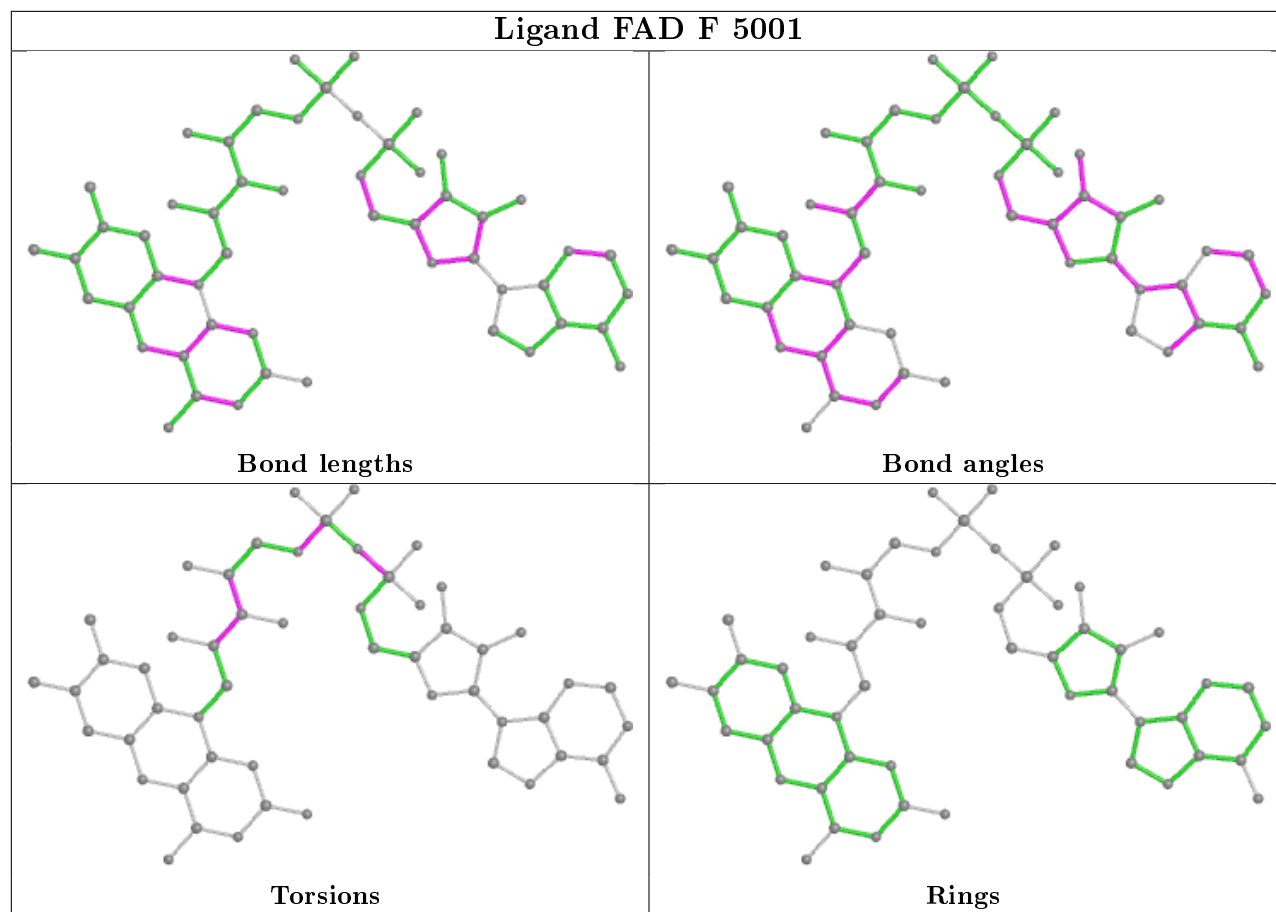
8 monomers are involved in 25 short contacts:

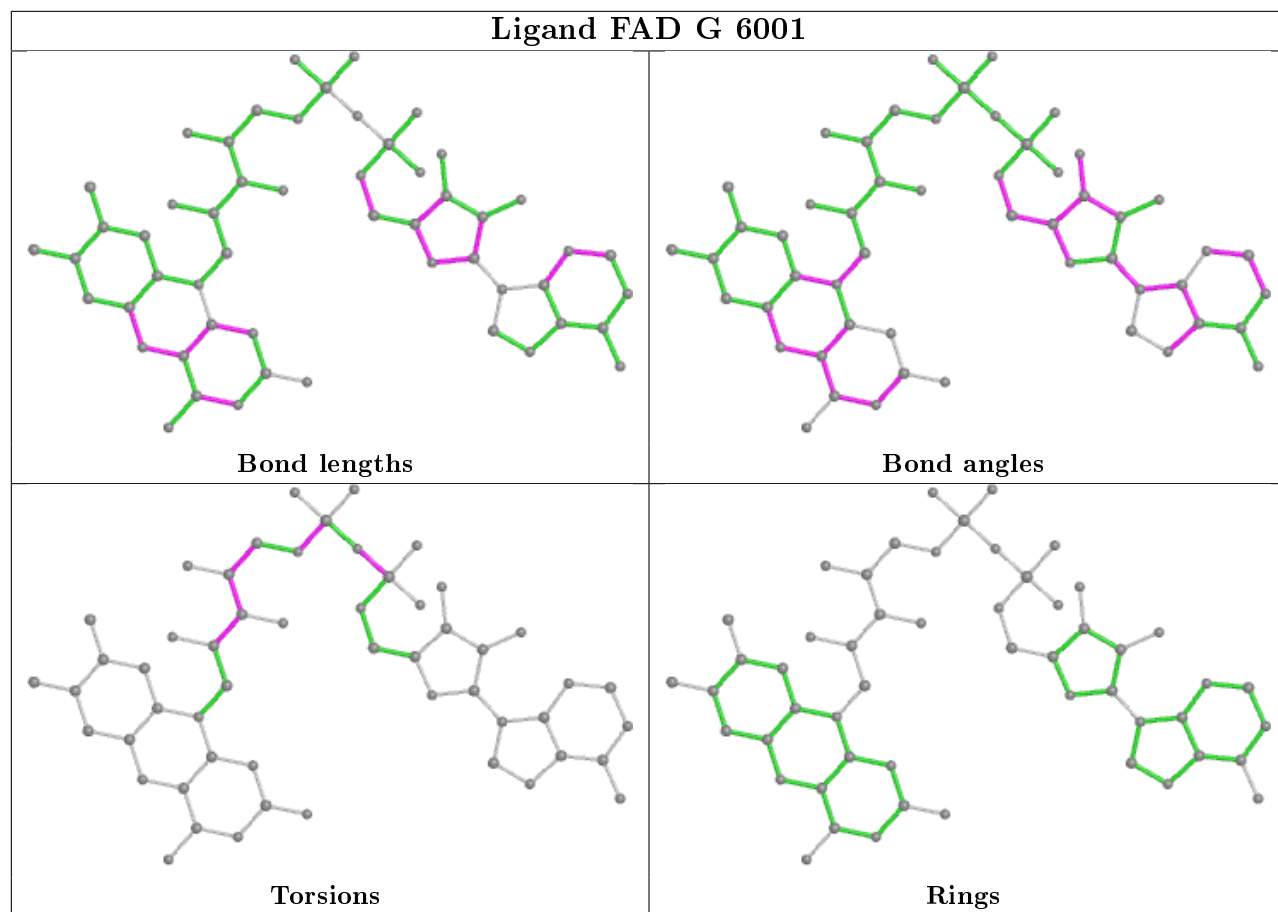
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3001	FAD	5	0
2	F	5001	FAD	2	0
2	G	6001	FAD	1	0
2	I	8001	FAD	4	0
2	H	7001	FAD	1	0
2	A	1001	FAD	4	0
2	C	2001	FAD	5	0
2	E	4001	FAD	3	0

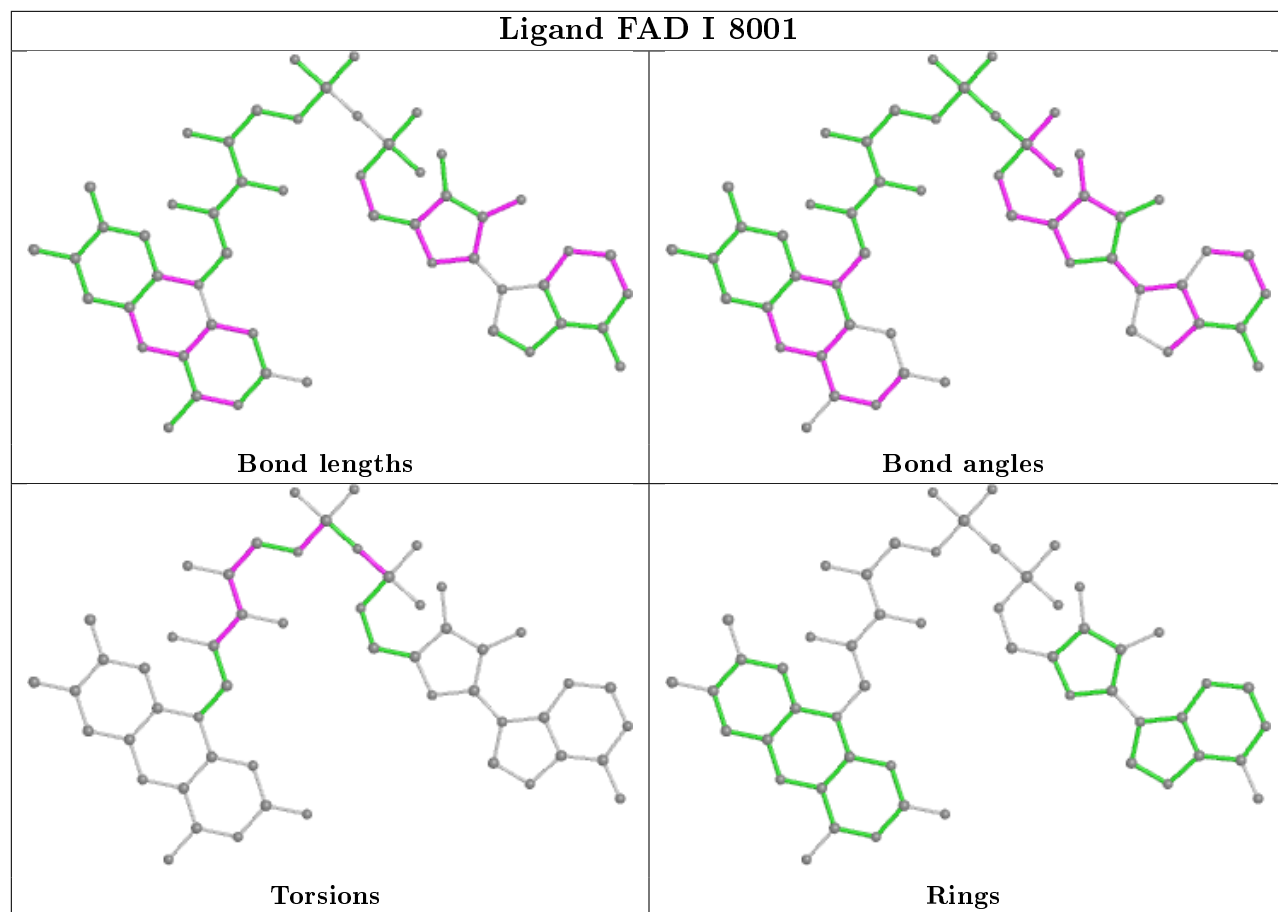
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

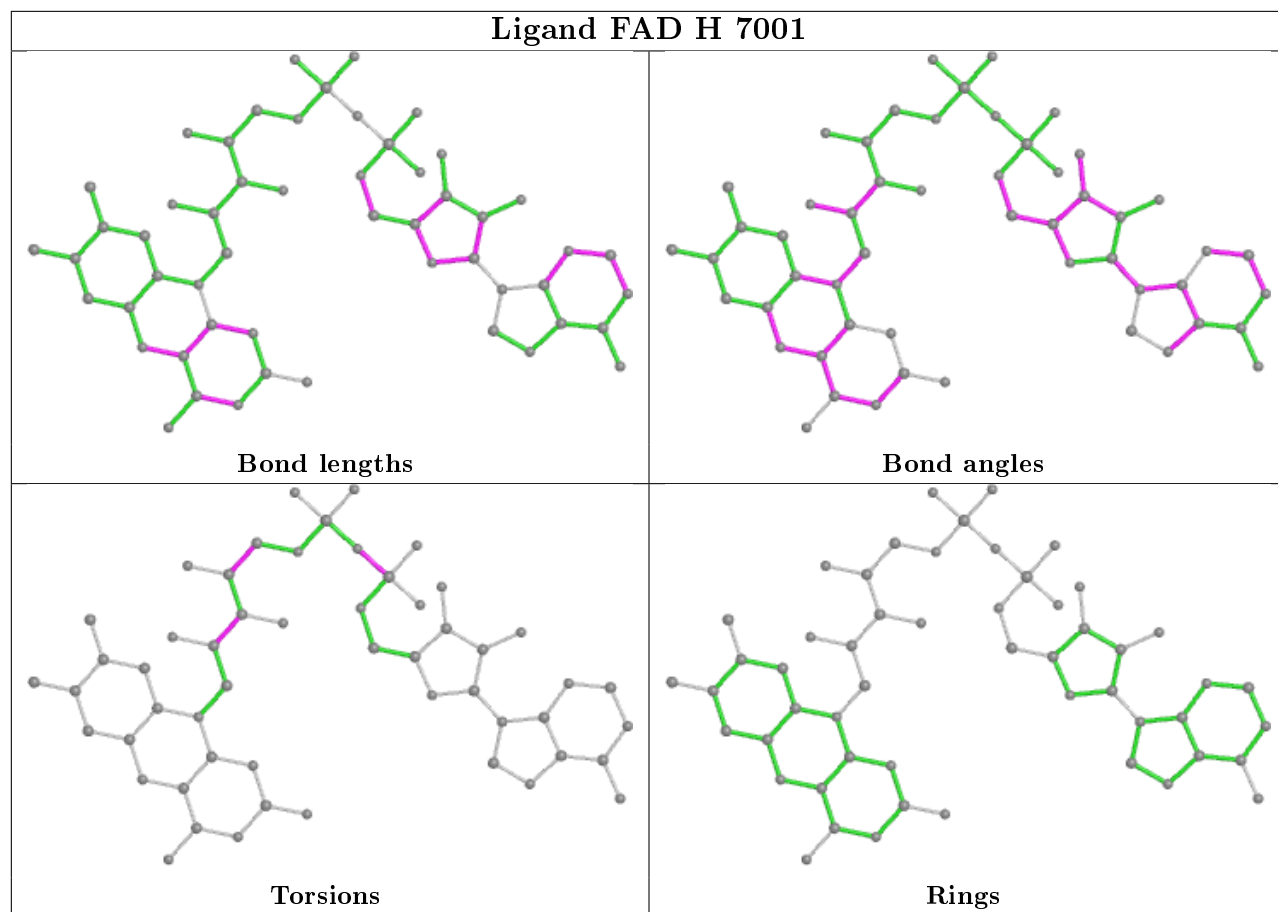
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

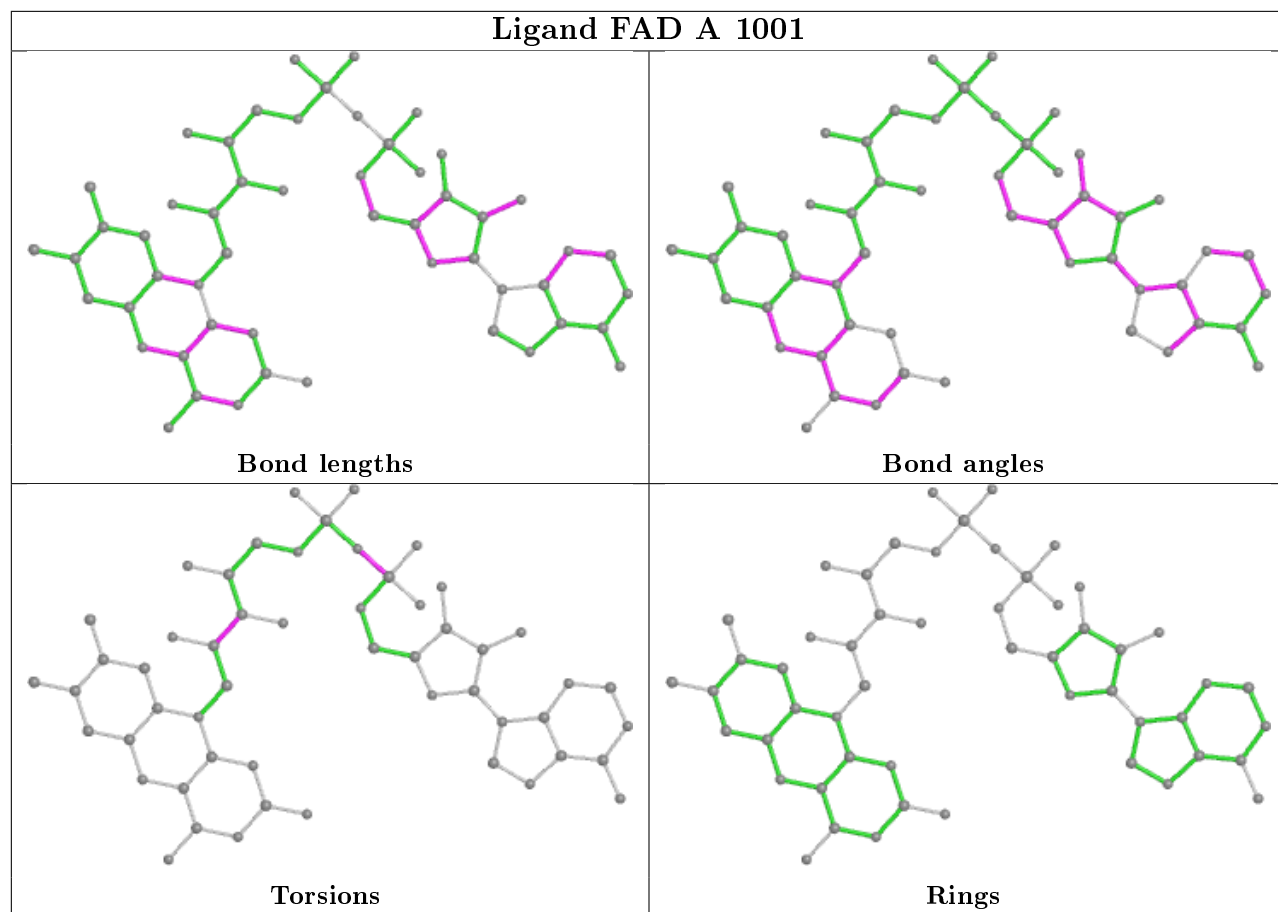


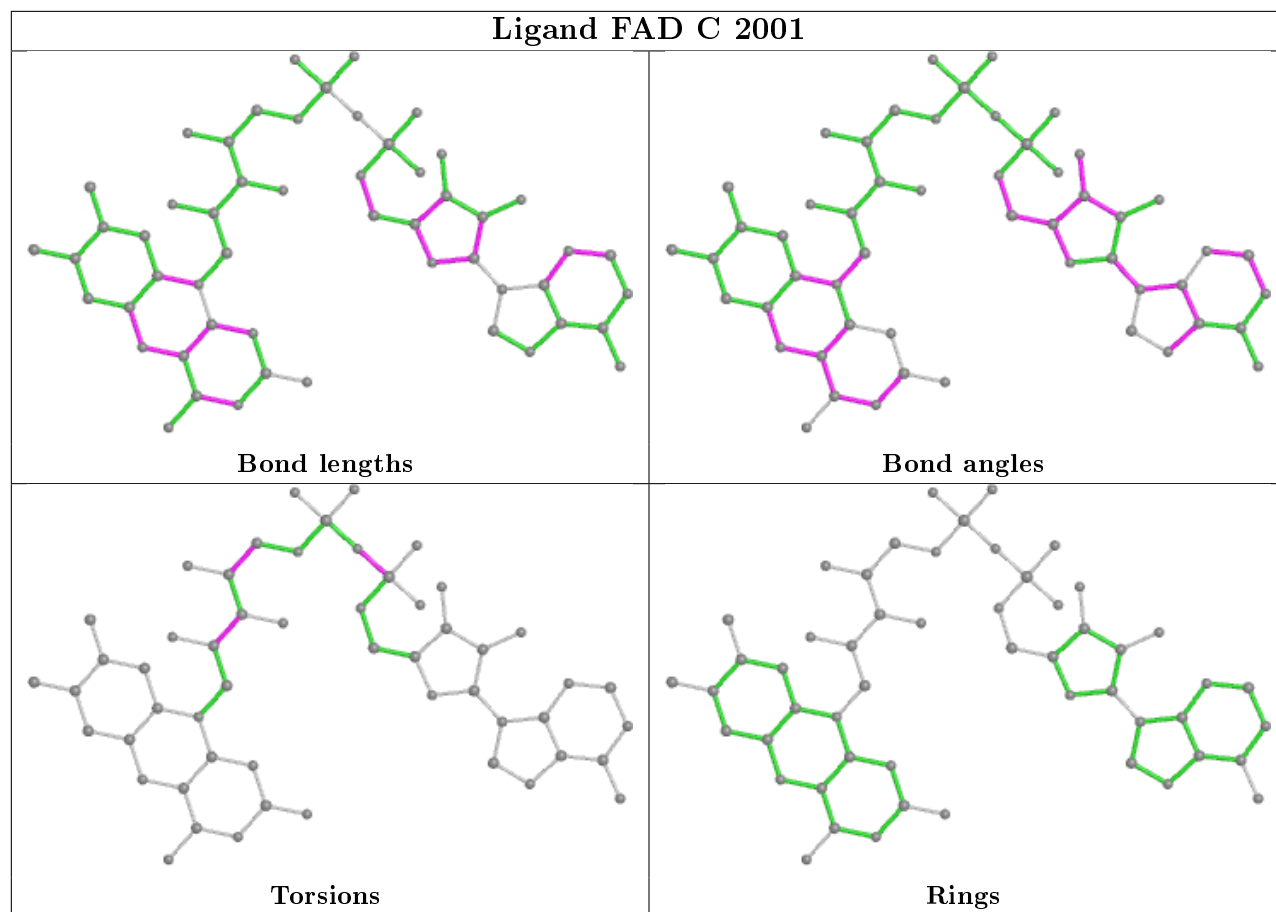


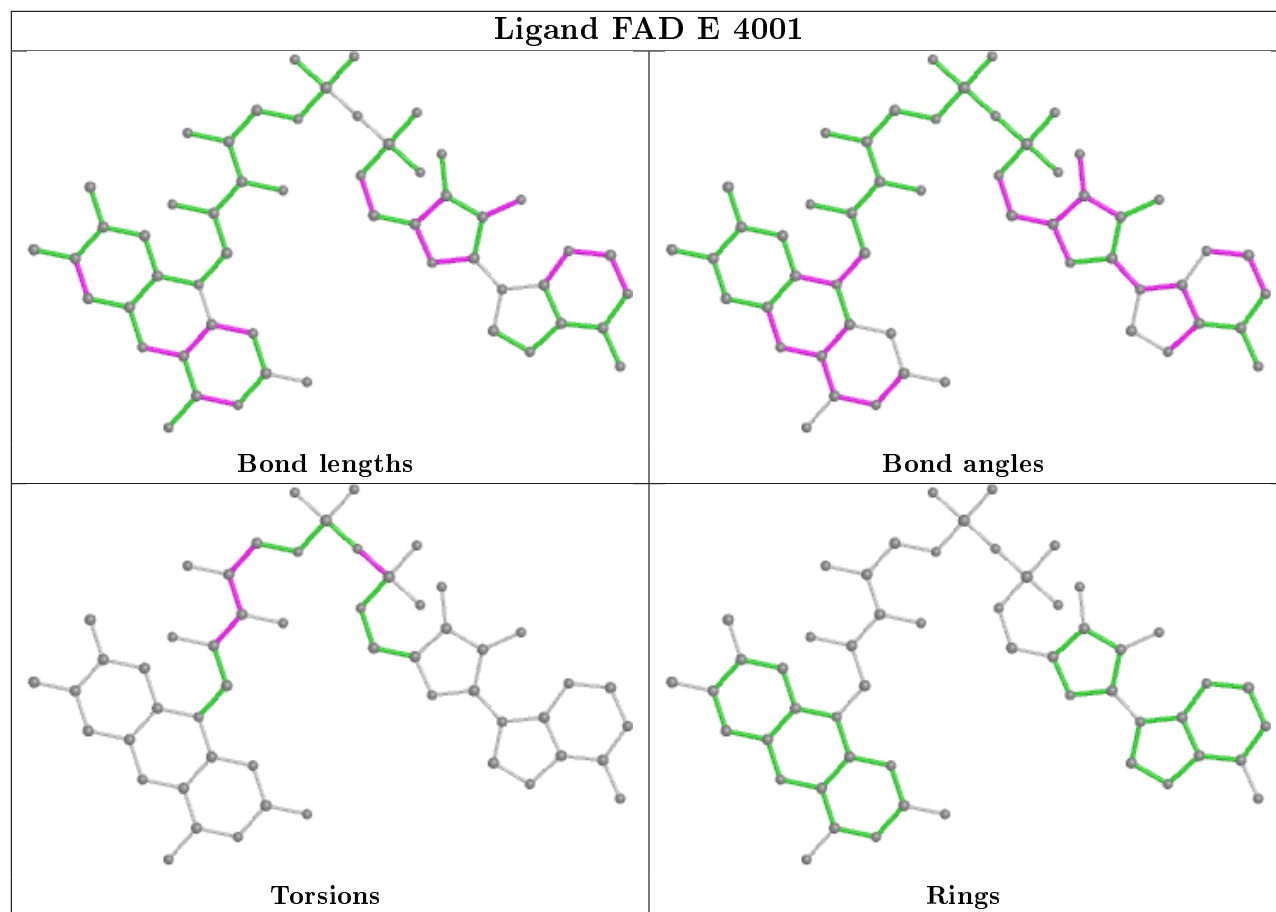












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å²)	Q<0.9	
1	A	380/385 (98%)	-0.82	0	100	100	7, 18, 31, 37	0
1	C	380/385 (98%)	-0.71	0	100	100	8, 19, 31, 37	0
1	D	380/385 (98%)	-0.76	0	100	100	7, 23, 33, 39	0
1	E	380/385 (98%)	-0.74	0	100	100	8, 23, 33, 39	0
1	F	380/385 (98%)	-0.65	1 (0%)	94	93	10, 24, 33, 40	0
1	G	380/385 (98%)	-0.85	0	100	100	8, 20, 31, 37	0
1	H	380/385 (98%)	-0.82	0	100	100	8, 19, 30, 37	0
1	I	380/385 (98%)	-0.81	1 (0%)	94	93	9, 22, 32, 40	0
All	All	3040/3080 (98%)	-0.77	2 (0%)	95	95	7, 21, 32, 40	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	232	LEU	2.5
1	F	195	GLY	2.2

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

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

6.3 Carbohydrates [i](#)

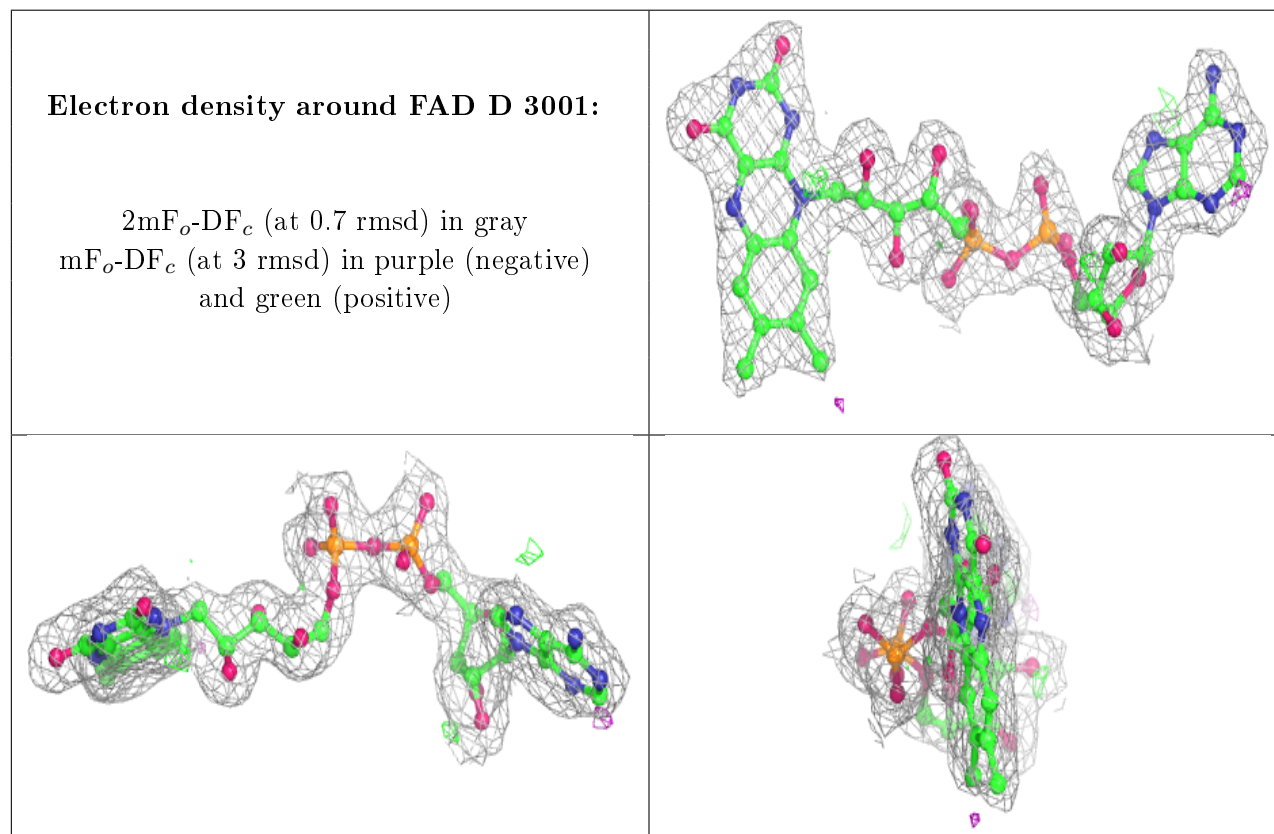
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

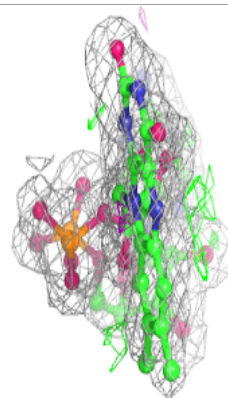
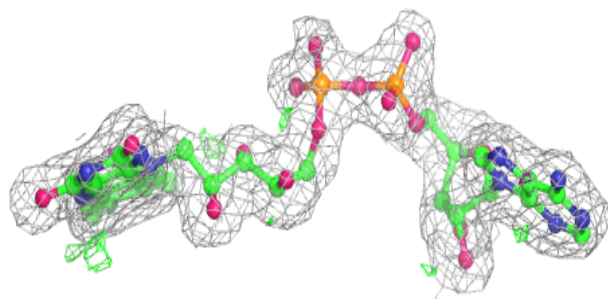
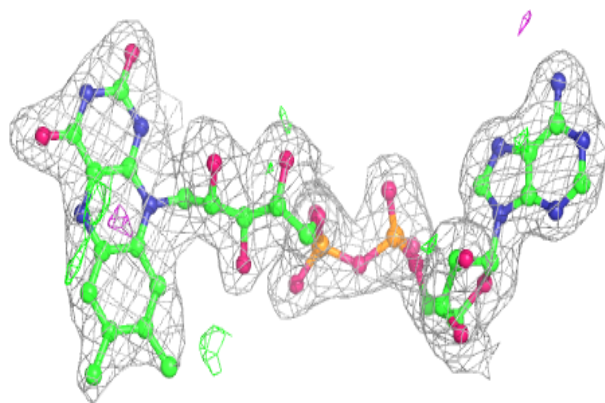
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FAD	D	3001	53/53	0.97	0.09	18,23,28,31	0
2	FAD	F	5001	53/53	0.97	0.09	18,24,29,30	0
2	FAD	I	8001	53/53	0.97	0.09	19,24,28,30	0
2	FAD	A	1001	53/53	0.97	0.10	15,20,22,23	0
2	FAD	C	2001	53/53	0.97	0.09	17,21,24,25	0
2	FAD	E	4001	53/53	0.97	0.08	19,26,30,32	0
2	FAD	H	7001	53/53	0.98	0.10	19,22,27,30	0
2	FAD	G	6001	53/53	0.98	0.09	16,23,26,27	0

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

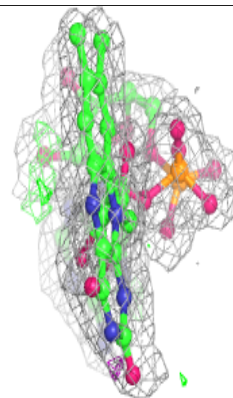
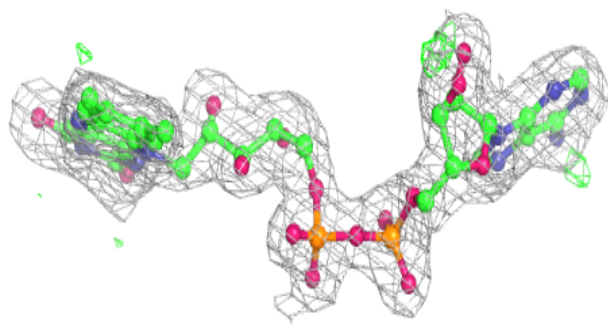
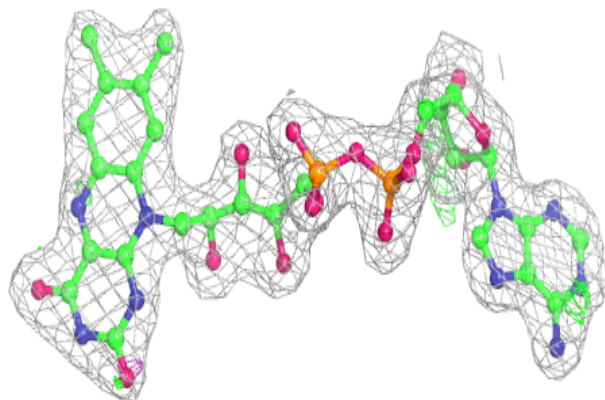


Electron density around FAD F 5001:

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

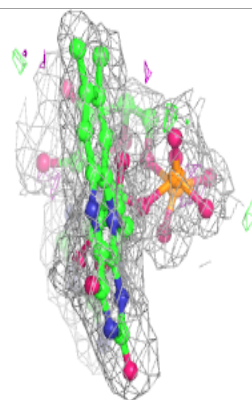
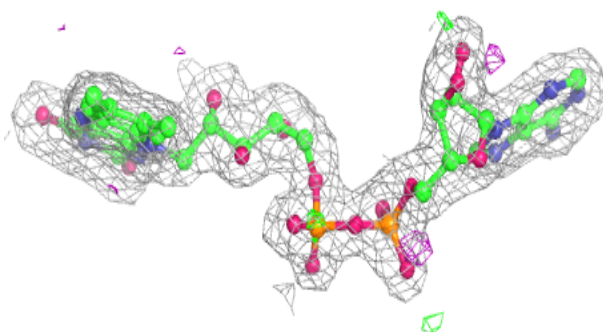
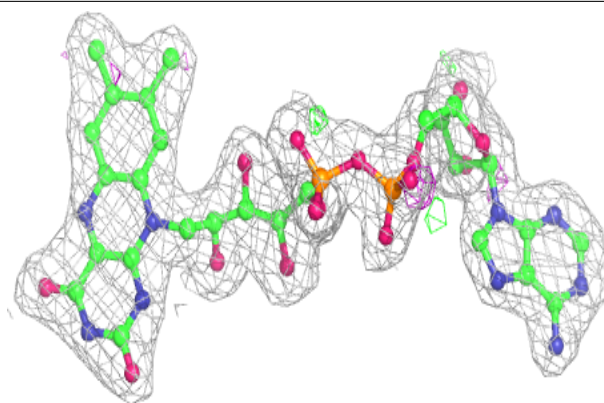
**Electron density around FAD I 8001:**

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

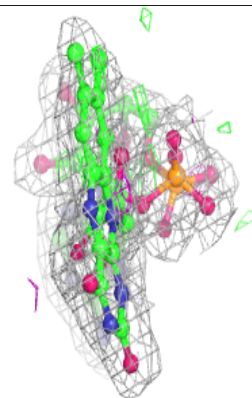
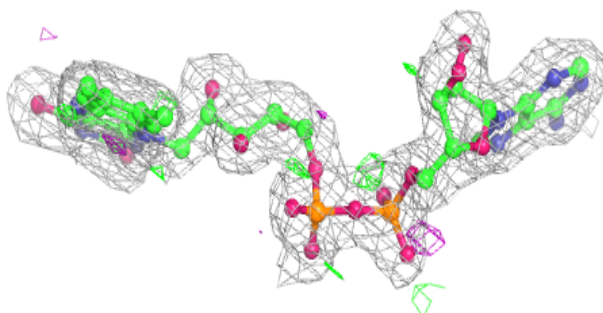
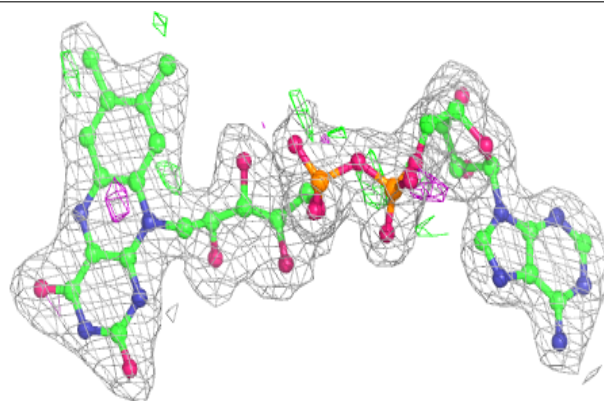


Electron density around FAD A 1001:

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

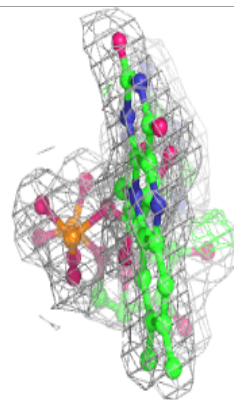
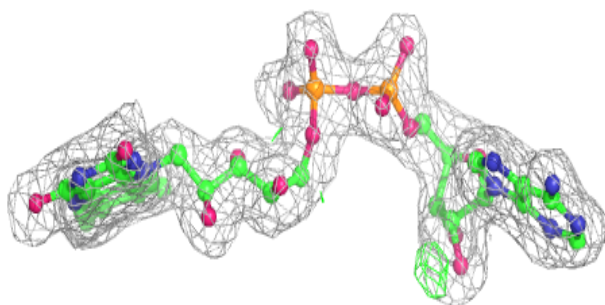
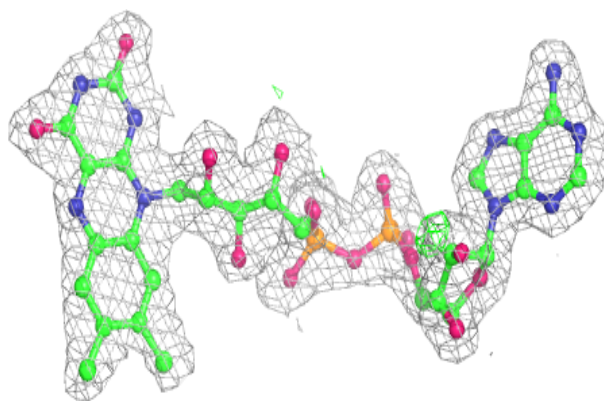
**Electron density around FAD C 2001:**

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

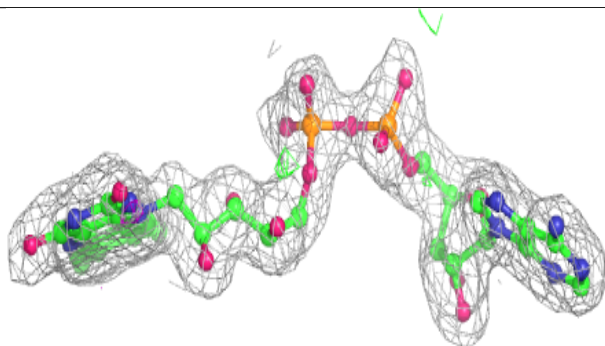
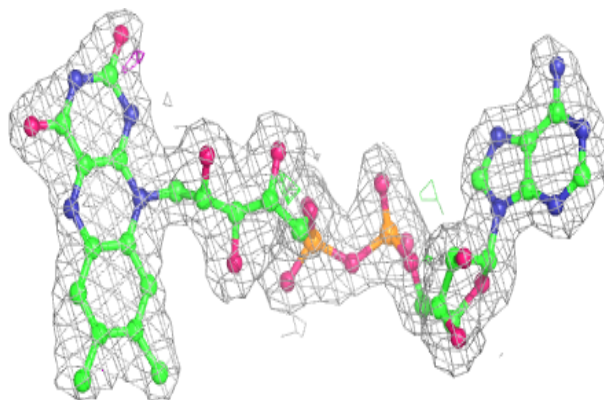


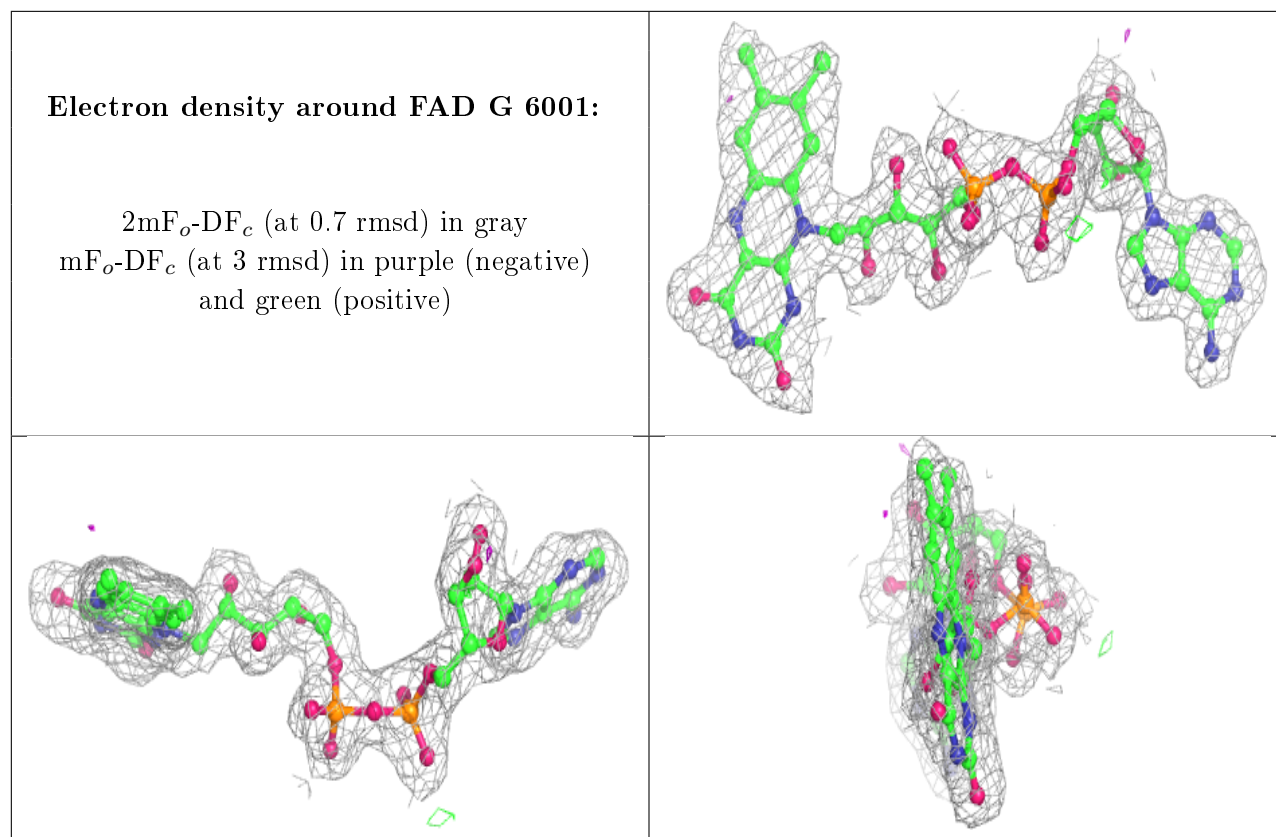
Electron density around FAD E 4001:

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

**Electron density around FAD H 7001:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.