



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:36 PM EDT

PDB ID : 3ZYV / pdb_00003zyv
Title : Crystal structure of the mouse liver Aldehyde Oxidase 3 (mAOX3)
Authors : Trincao, J.; Coelho, C.; Mahro, M.; Rodrigues, D.; Terao, M.; Garattini, E.;
Leimkuehler, S.; Romao, M.J.
Deposited on : 2011-08-27
Resolution : 2.54 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

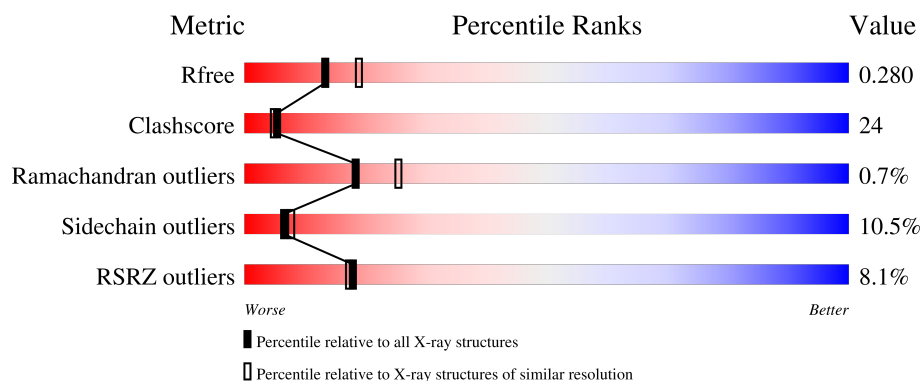
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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))
R_{free}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1335	7% 56% 33% 5% 6%
1	B	1335	7% 56% 33% 5% 5%
1	C	1335	7% 57% 31% 5% 7%
1	D	1335	9% 56% 33% 5% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FES	D	3002	-	-	X	-
5	MOS	A	3004	-	-	X	-
5	MOS	B	3004	-	-	X	-
5	MOS	C	3004	-	-	X	-
5	MOS	D	3004	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 38315 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 AOX3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1253	Total	C	N	O	S	0	0	0
			9314	5905	1602	1747	60			
1	B	1262	Total	C	N	O	S	0	0	0
			9471	6016	1621	1774	60			
1	C	1244	Total	C	N	O	S	0	0	0
			9231	5865	1579	1728	59			
1	D	1257	Total	C	N	O	S	0	0	0
			9289	5892	1602	1739	56			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

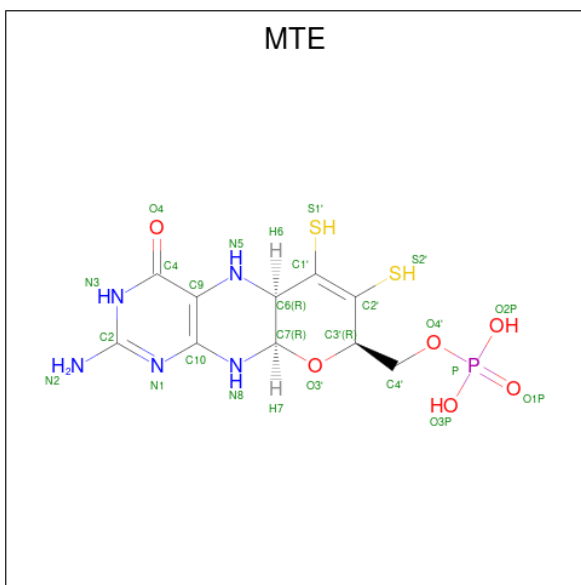
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



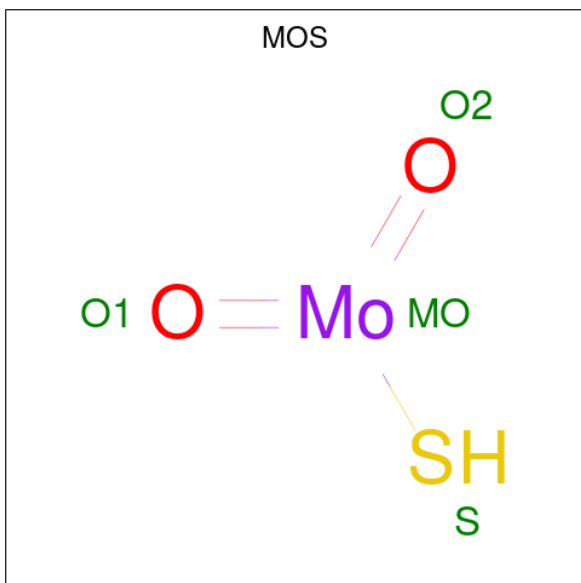
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (CCD ID: MTE) (formula: C₁₀H₁₄N₅O₆PS₂).



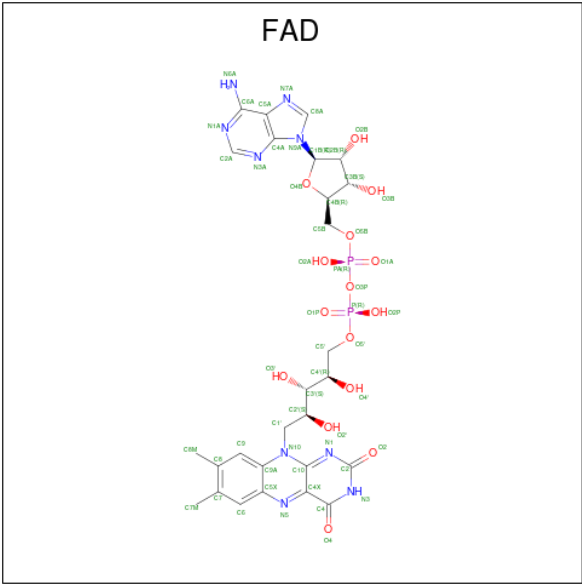
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (CCD ID: MOS) (formula: HMoO_2S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	B	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	C	1	Total	Mo	O	S	0	0
			4	1	2	1		
5	D	1	Total	Mo	O	S	0	0
			4	1	2	1		

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



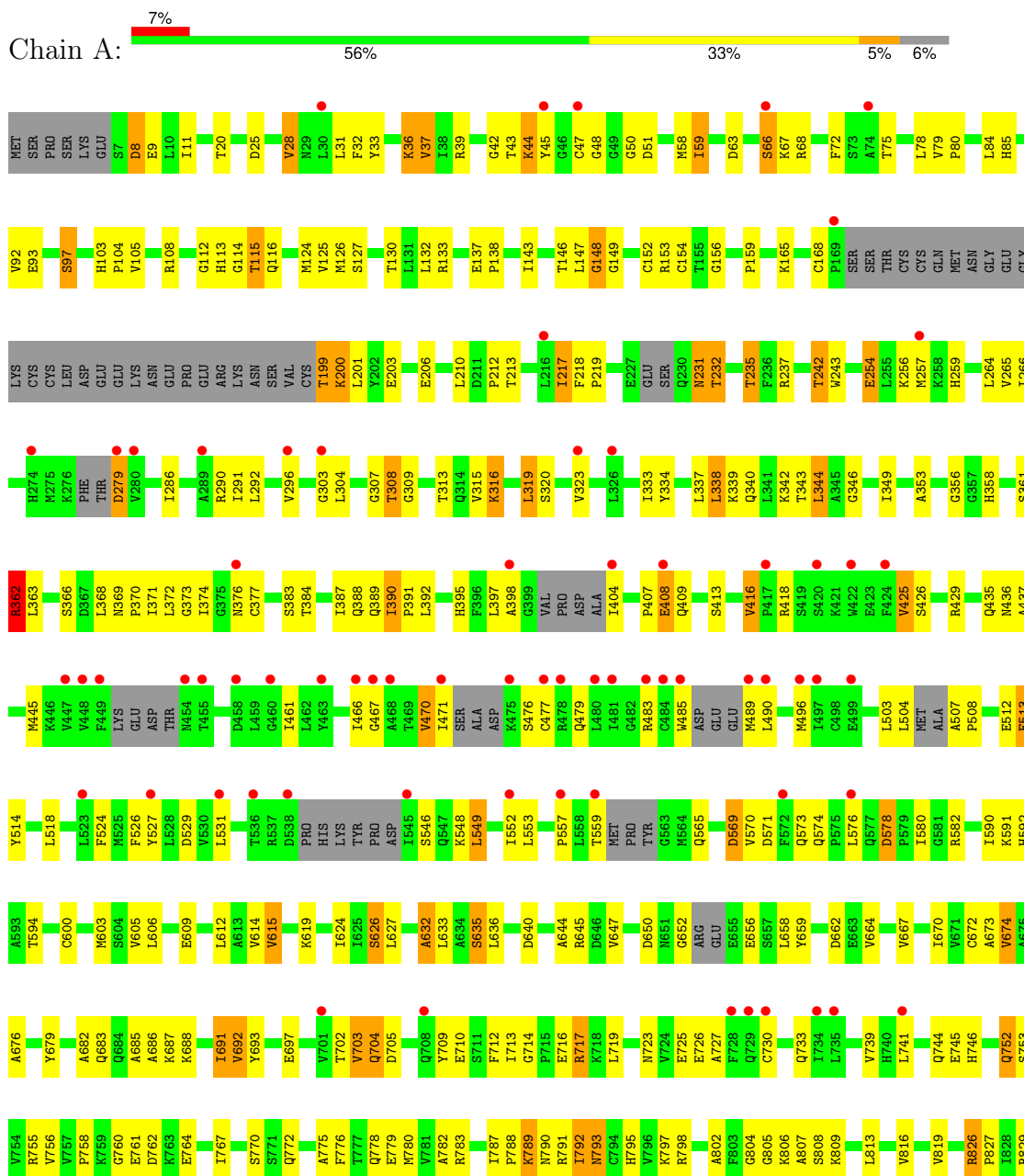
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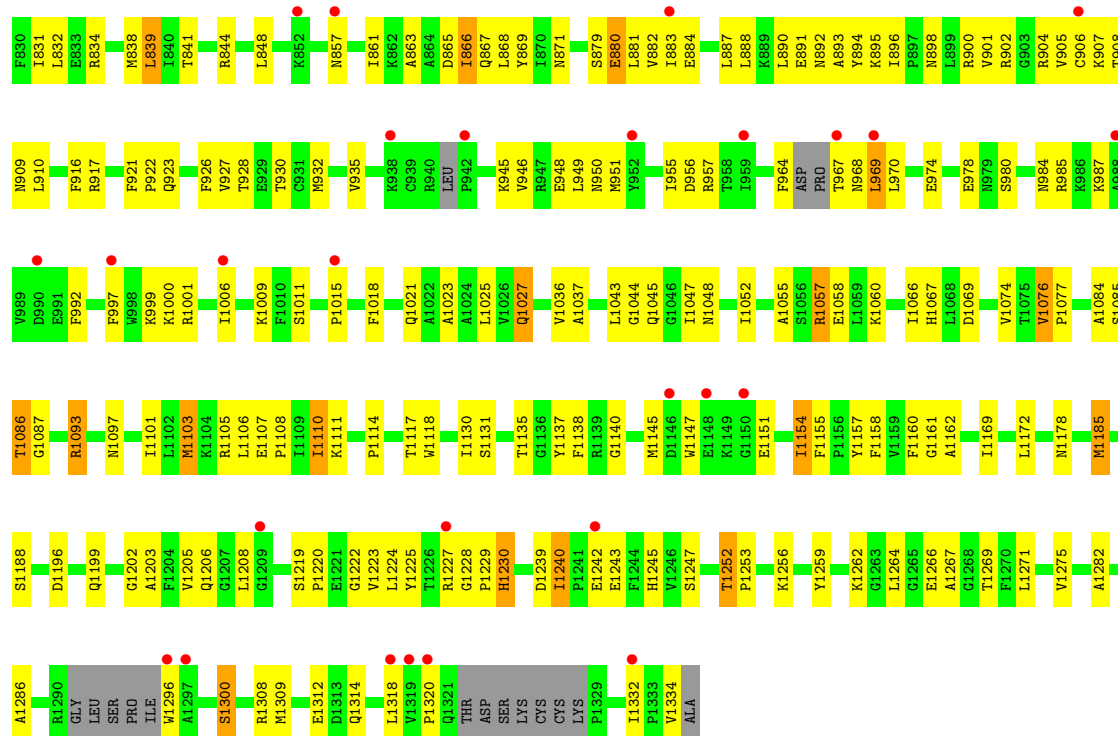
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	147	Total 147	O 147	0	0
7	D	155	Total 155	O 155	0	0

3 Residue-property plots

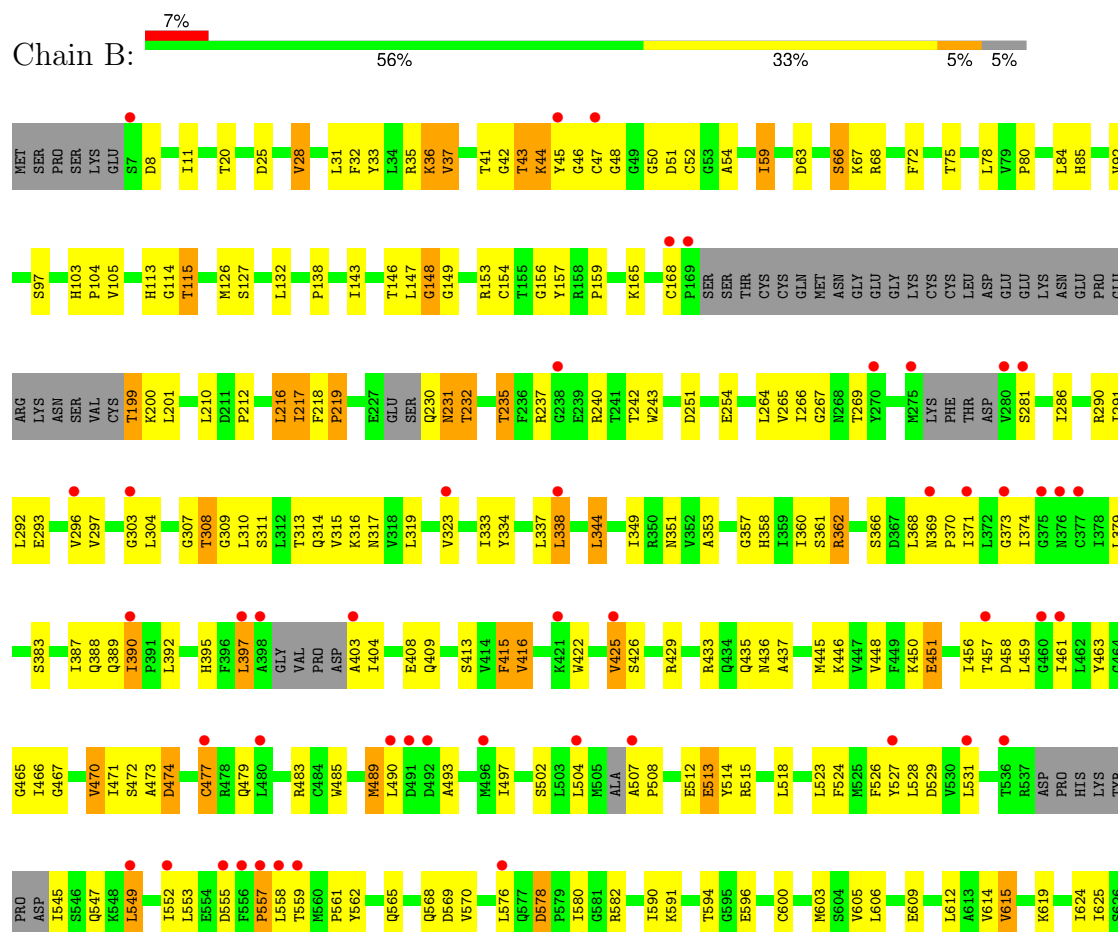
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

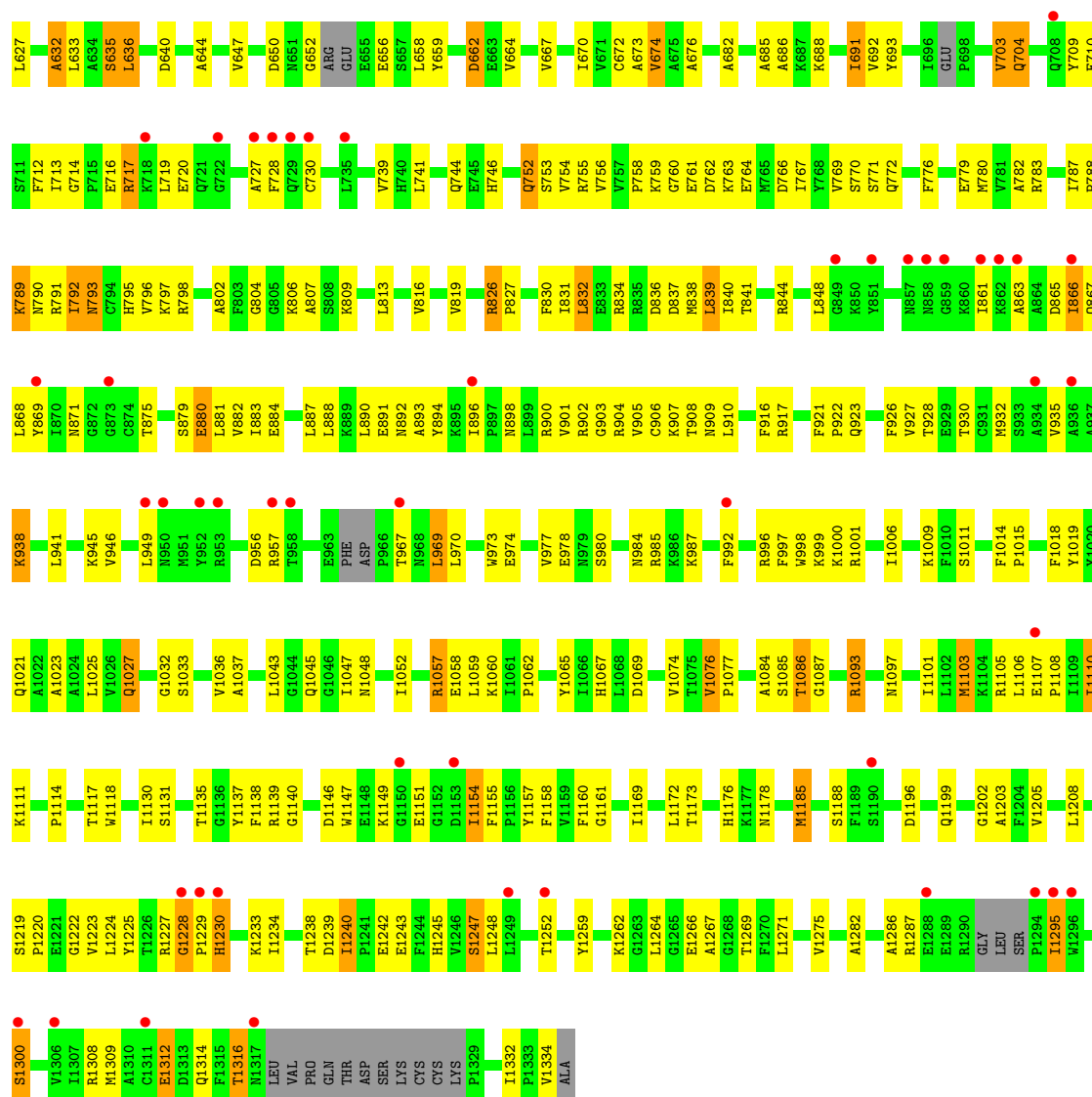
• Molecule 1: AOX3



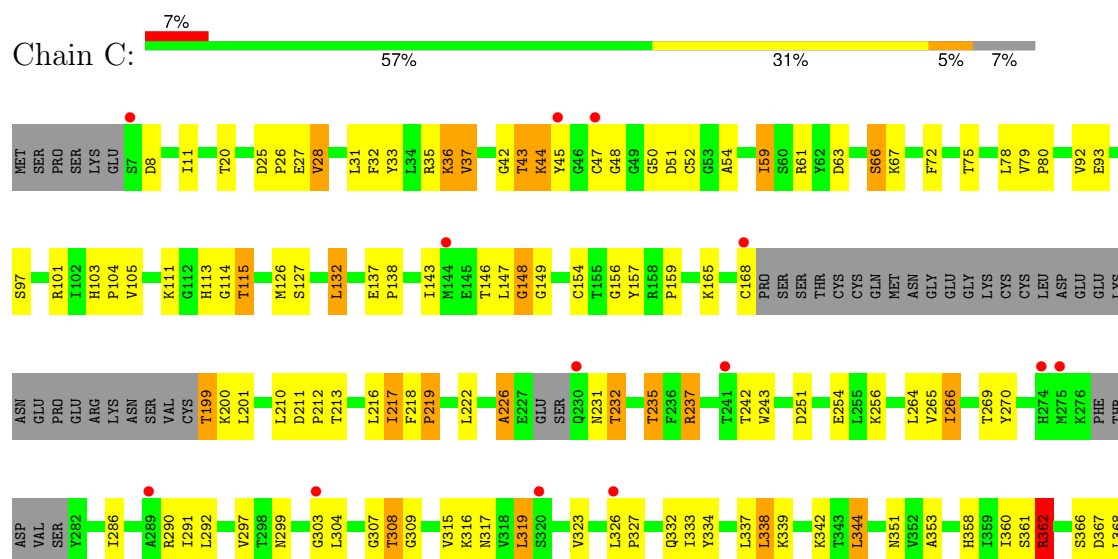


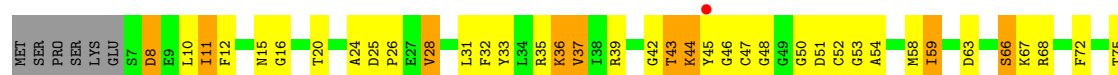
Chain B:

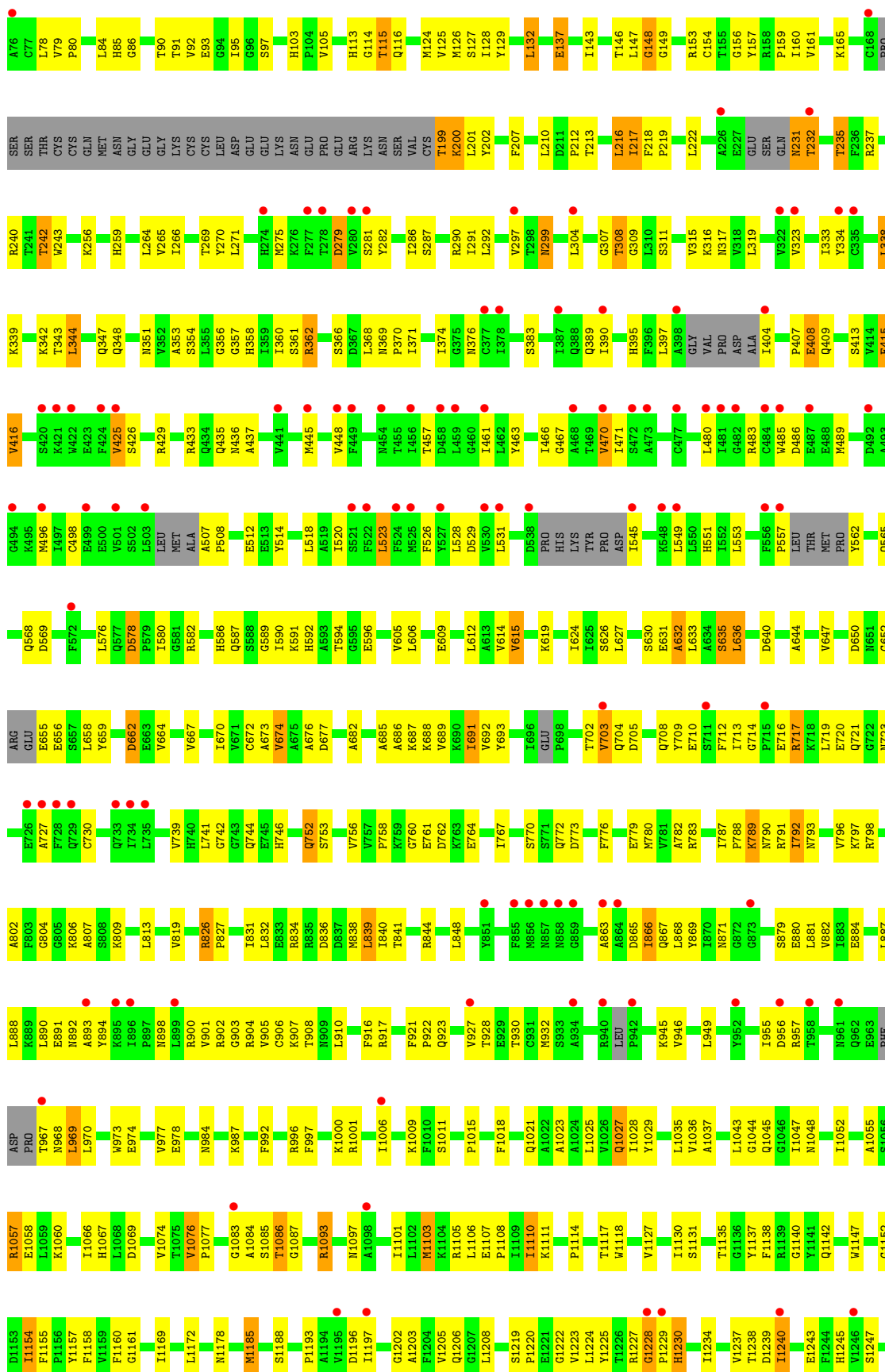


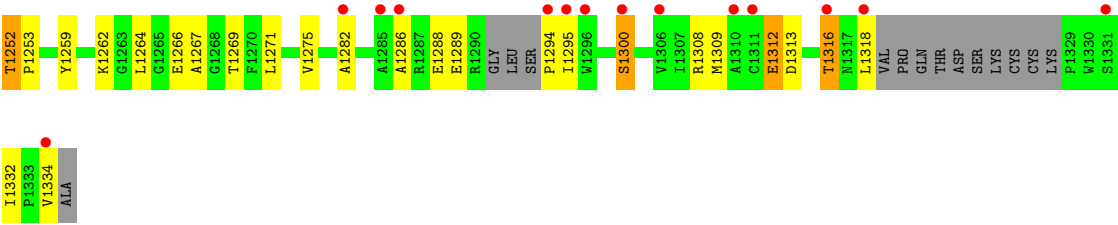


- Molecule 1: AOX3









4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 135.27Å 147.37Å 78.16° 77.72° 89.90°	Depositor
Resolution (Å)	49.91 – 2.54 49.91 – 2.54	Depositor EDS
% Data completeness (in resolution range)	75.0 (49.91-2.54) 75.0 (49.91-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.285 0.251 , 0.280	Depositor DCC
R_{free} test set	8336 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 69.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	38315	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, NA, MTE, FES, MOS

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	0.40	0/9482	0.81	14/12869 (0.1%)
1	B	0.40	0/9650	0.82	16/13097 (0.1%)
1	C	0.39	0/9398	0.81	14/12757 (0.1%)
1	D	0.40	0/9460	0.80	12/12852 (0.1%)
All	All	0.40	0/37990	0.81	56/51575 (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	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	941	LEU	CA-C-N	10.62	131.32	120.38
1	B	941	LEU	C-N-CA	10.62	131.32	120.38
1	B	826	ARG	N-CA-C	8.57	115.70	108.07
1	C	619	LYS	CB-CG-CD	8.54	130.95	111.30
1	B	558	LEU	N-CA-C	-8.30	93.99	108.69
1	C	226	ALA	N-CA-C	7.43	122.41	113.12
1	D	826	ARG	N-CA-C	7.40	114.66	108.07
1	A	826	ARG	N-CA-C	7.38	114.64	108.07
1	C	826	ARG	N-CA-C	7.24	114.52	108.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	561	PRO	N-CA-CB	6.78	109.37	103.27
1	A	697	GLU	C-N-CD	-6.60	106.07	120.60
1	A	697	GLU	CA-C-N	6.40	142.36	127.00
1	A	697	GLU	C-N-CA	6.40	142.36	127.00
1	A	697	GLU	N-CA-C	-6.40	101.71	109.83
1	C	37	VAL	N-CA-C	6.08	116.83	111.90
1	B	1076	VAL	CA-C-N	6.01	126.20	120.31
1	B	1076	VAL	C-N-CA	6.01	126.20	120.31
1	A	37	VAL	N-CA-C	5.93	116.66	111.56
1	C	1300	SER	CA-C-N	-5.92	112.44	119.84
1	C	1300	SER	C-N-CA	-5.92	112.44	119.84
1	D	37	VAL	N-CA-C	5.91	116.64	111.56
1	B	37	VAL	N-CA-C	5.88	116.61	111.56
1	A	1300	SER	CA-C-N	-5.71	112.70	119.84
1	A	1300	SER	C-N-CA	-5.71	112.70	119.84
1	B	1300	SER	CA-C-N	-5.69	112.72	119.84
1	B	1300	SER	C-N-CA	-5.69	112.72	119.84
1	B	1228	GLY	CA-C-N	5.67	125.03	118.85
1	B	1228	GLY	C-N-CA	5.67	125.03	118.85
1	C	137	GLU	CA-C-N	5.59	126.07	120.14
1	C	137	GLU	C-N-CA	5.59	126.07	120.14
1	D	1300	SER	CA-C-N	-5.58	112.87	119.84
1	D	1300	SER	C-N-CA	-5.58	112.87	119.84
1	A	1228	GLY	CA-C-N	5.54	125.19	119.05
1	A	1228	GLY	C-N-CA	5.54	125.19	119.05
1	A	1076	VAL	CA-C-N	5.52	125.99	120.14
1	A	1076	VAL	C-N-CA	5.52	125.99	120.14
1	D	1228	GLY	CA-C-N	5.49	125.14	119.05
1	D	1228	GLY	C-N-CA	5.49	125.14	119.05
1	D	1076	VAL	CA-C-N	5.47	125.68	120.31
1	D	1076	VAL	C-N-CA	5.47	125.68	120.31
1	B	219	PRO	CA-C-N	5.39	125.21	119.28
1	B	219	PRO	C-N-CA	5.39	125.21	119.28
1	C	1076	VAL	CA-C-N	5.33	125.78	120.14
1	C	1076	VAL	C-N-CA	5.33	125.78	120.14
1	C	473	ALA	N-CA-C	-5.28	106.86	113.15
1	C	619	LYS	CG-CD-CE	5.24	123.35	111.30
1	A	219	PRO	CA-C-N	5.21	125.01	119.28
1	A	219	PRO	C-N-CA	5.21	125.01	119.28
1	C	219	PRO	CA-C-N	5.14	124.94	119.28
1	C	219	PRO	C-N-CA	5.14	124.94	119.28
1	B	896	ILE	CA-C-N	5.12	125.41	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	896	ILE	C-N-CA	5.12	125.41	119.47
1	D	219	PRO	CA-C-N	5.04	124.82	119.28
1	D	219	PRO	C-N-CA	5.04	124.82	119.28
1	D	137	GLU	CA-C-N	5.04	125.48	120.14
1	D	137	GLU	C-N-CA	5.04	125.48	120.14

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	557	PRO	Peptide
1	B	557	PRO	Peptide
1	C	226	ALA	Peptide

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	9314	0	9046	454	0
1	B	9471	0	9271	465	0
1	C	9231	0	8962	429	0
1	D	9289	0	8958	462	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	8	0	0	1	0
3	B	8	0	0	1	0
3	C	8	0	0	1	0
3	D	8	0	0	2	0
4	A	24	0	10	4	0
4	B	24	0	10	1	0
4	C	24	0	10	3	0
4	D	24	0	10	3	0
5	A	4	0	0	2	0
5	B	4	0	0	2	0
5	C	4	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	4	0	0	2	0
6	A	53	0	31	8	0
6	B	53	0	31	14	0
6	C	53	0	31	20	0
6	D	53	0	31	15	0
7	A	182	0	0	93	0
7	B	166	0	0	67	0
7	C	147	0	0	56	0
7	D	155	0	0	92	0
All	All	38315	0	36401	1775	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (1775) 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)
6:B:3005:FAD:H9	6:B:3005:FAD:O2'	1.48	1.12
1:A:308:THR:HG21	6:A:3005:FAD:N6A	1.62	1.11
1:B:308:THR:HG21	6:B:3005:FAD:N6A	1.67	1.09
1:A:496:MET:SD	7:A:2076:HOH:O	2.12	1.07
1:D:12:PHE:HB3	7:D:2002:HOH:O	1.55	1.06
1:A:58:MET:SD	7:A:2015:HOH:O	2.18	1.02
1:C:986:LYS:N	7:C:2114:HOH:O	1.90	1.02
1:D:655:GLU:N	7:D:2095:HOH:O	1.95	1.00
1:D:807:ALA:O	7:D:2111:HOH:O	1.81	0.98
1:A:713:ILE:HG13	1:A:907:LYS:HB3	1.46	0.97
1:D:714:GLY:O	1:D:904:ARG:NH1	1.98	0.96
1:D:713:ILE:HG13	1:D:907:LYS:HB3	1.46	0.96
1:B:713:ILE:HG13	1:B:907:LYS:HB3	1.47	0.96
1:D:562:TYR:N	7:D:2079:HOH:O	1.97	0.96
6:C:3005:FAD:H2'	6:C:3005:FAD:H9	1.44	0.95
1:A:714:GLY:O	1:A:904:ARG:NH1	2.00	0.95
1:C:993:ASN:O	7:C:2115:HOH:O	1.83	0.94
1:B:714:GLY:O	1:B:904:ARG:NH1	2.00	0.94
1:C:1024:ALA:N	7:C:2119:HOH:O	2.00	0.94
1:D:496:MET:SD	7:D:2074:HOH:O	2.25	0.93
1:D:1219:SER:N	7:D:2148:HOH:O	2.01	0.93
1:D:11:ILE:O	7:D:2002:HOH:O	1.88	0.92
1:A:9:GLU:OE2	7:A:2003:HOH:O	1.88	0.92
6:B:3005:FAD:H8A	6:B:3005:FAD:H52A	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1093:ARG:HH11	1:B:1093:ARG:CG	1.84	0.91
1:B:1247:SER:O	7:B:2158:HOH:O	1.89	0.91
1:B:216:LEU:H	1:B:216:LEU:HD12	1.33	0.91
1:D:72:PHE:O	7:D:2013:HOH:O	1.90	0.90
1:A:565:GLN:NE2	7:A:2035:HOH:O	2.05	0.90
1:B:771:SER:N	7:B:2115:HOH:O	2.04	0.89
1:C:890:LEU:HD21	1:C:901:VAL:HG21	1.55	0.89
1:C:1093:ARG:CG	1:C:1093:ARG:HH11	1.85	0.89
1:A:201:LEU:HD11	1:A:565:GLN:HG3	1.54	0.88
1:C:397:LEU:HD22	1:C:470:VAL:HG21	1.56	0.88
1:D:890:LEU:HD21	1:D:901:VAL:HG21	1.54	0.88
1:D:1093:ARG:HH11	1:D:1093:ARG:CG	1.86	0.88
1:C:505:MET:CB	1:C:506:ALA:HA	2.03	0.88
1:B:837:ASP:OD1	7:B:2110:HOH:O	1.90	0.88
1:A:308:THR:HG21	6:A:3005:FAD:H61A	1.35	0.87
1:A:1093:ARG:CG	1:A:1093:ARG:HH11	1.86	0.87
1:B:890:LEU:HD21	1:B:901:VAL:HG21	1.56	0.87
1:A:692:VAL:O	7:A:2105:HOH:O	1.92	0.87
1:D:1289:GLU:O	7:D:2152:HOH:O	1.91	0.87
1:A:890:LEU:HD21	1:A:901:VAL:HG21	1.56	0.87
6:C:3005:FAD:H2'	6:C:3005:FAD:C9	2.01	0.87
1:B:752:GLN:HG2	1:B:813:LEU:HD12	1.57	0.86
1:C:596:GLU:OE1	7:C:2075:HOH:O	1.93	0.86
1:C:237:ARG:O	7:C:2003:HOH:O	1.94	0.86
1:C:31:LEU:HD21	1:C:45:TYR:HB3	1.57	0.86
1:D:650:ASP:OD2	1:D:783:ARG:NH1	2.07	0.86
1:D:723:ASN:ND2	7:D:2105:HOH:O	2.06	0.86
1:C:752:GLN:HG2	1:C:813:LEU:HD12	1.58	0.86
1:B:1033:SER:HA	7:B:2141:HOH:O	1.76	0.85
1:A:679:TYR:OH	7:A:2118:HOH:O	1.92	0.85
1:D:752:GLN:HG2	1:D:813:LEU:HD12	1.57	0.85
1:A:650:ASP:OD2	1:A:783:ARG:NH1	2.09	0.85
1:A:264:LEU:O	6:A:3005:FAD:H2B	1.76	0.85
1:B:650:ASP:OD2	1:B:783:ARG:NH1	2.08	0.84
1:B:741:LEU:HG	1:B:1300:SER:HB2	1.60	0.84
1:B:769:VAL:C	7:B:2115:HOH:O	2.19	0.84
1:A:752:GLN:HG2	1:A:813:LEU:HD12	1.57	0.84
1:A:31:LEU:HD21	1:A:45:TYR:HB3	1.58	0.84
1:B:1222:GLY:O	7:B:2103:HOH:O	1.95	0.83
1:D:773:ASP:HA	7:D:2112:HOH:O	1.76	0.83
1:C:505:MET:HB3	1:C:506:ALA:HA	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:CYS:O	7:A:2032:HOH:O	1.95	0.83
1:A:967:THR:N	7:A:2146:HOH:O	2.11	0.83
1:D:968:ASN:ND2	7:D:2125:HOH:O	2.10	0.83
1:C:251:ASP:OD1	7:C:2043:HOH:O	1.96	0.83
1:C:1077:PRO:HG3	1:D:1027:GLN:HG3	1.59	0.83
1:A:741:LEU:HG	1:A:1300:SER:HB2	1.61	0.83
1:B:201:LEU:HD11	1:B:565:GLN:HG3	1.59	0.83
1:C:741:LEU:HG	1:C:1300:SER:HB2	1.60	0.83
1:D:1312:GLU:HB3	1:D:1316:THR:HG21	1.61	0.83
1:A:476:SER:HA	7:A:2076:HOH:O	1.78	0.82
1:C:485:TRP:NE1	7:C:2066:HOH:O	2.12	0.82
1:D:31:LEU:HD21	1:D:45:TYR:HB3	1.60	0.82
1:C:704:GLN:H	1:C:704:GLN:HE21	1.28	0.82
1:B:483:ARG:NH1	7:B:2069:HOH:O	2.11	0.82
1:D:568:GLN:NE2	7:D:2082:HOH:O	2.11	0.82
1:D:1294:PRO:O	7:D:2153:HOH:O	1.98	0.82
1:B:308:THR:HG21	6:B:3005:FAD:H61A	1.45	0.81
1:B:766:ASP:OD1	7:B:2112:HOH:O	1.96	0.81
7:C:2100:HOH:O	1:D:797:LYS:NZ	2.08	0.81
1:B:31:LEU:HD21	1:B:45:TYR:HB3	1.60	0.81
1:C:308:THR:HG21	6:C:3005:FAD:H61A	1.44	0.81
1:A:308:THR:HG23	7:A:2058:HOH:O	1.80	0.81
1:A:308:THR:O	7:A:2058:HOH:O	1.97	0.81
1:C:983:TYR:C	7:C:2114:HOH:O	2.22	0.81
1:A:1199:GLN:OE1	7:A:2170:HOH:O	1.99	0.80
1:C:397:LEU:HD22	1:C:470:VAL:CG2	2.12	0.80
1:D:308:THR:HG23	7:D:2057:HOH:O	1.79	0.80
1:C:650:ASP:OD2	1:C:783:ARG:NH1	2.13	0.80
1:D:269:THR:HG1	6:D:3005:FAD:HO3'	0.86	0.80
1:C:266:ILE:HA	7:C:2044:HOH:O	1.81	0.80
6:C:3005:FAD:H9	6:C:3005:FAD:C2'	2.11	0.80
1:D:58:MET:HG3	7:D:2013:HOH:O	1.80	0.80
1:D:1093:ARG:NH1	7:D:2137:HOH:O	2.14	0.80
1:C:379:LEU:O	7:C:2060:HOH:O	2.00	0.80
1:D:58:MET:O	7:D:2012:HOH:O	1.99	0.79
1:D:631:GLU:OE1	7:D:2090:HOH:O	1.99	0.79
1:D:24:ALA:HB1	7:D:2020:HOH:O	1.83	0.79
1:D:1223:VAL:N	7:D:2148:HOH:O	2.15	0.79
1:C:201:LEU:HD11	1:C:565:GLN:HG3	1.62	0.79
1:C:1094:ALA:HB1	7:C:2119:HOH:O	1.80	0.79
1:A:752:GLN:NE2	7:A:2128:HOH:O	1.91	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:SER:OG	7:D:2069:HOH:O	2.00	0.79
1:A:867:GLN:OE1	1:A:869:TYR:OH	2.01	0.79
1:B:967:THR:HG22	7:B:2131:HOH:O	1.83	0.78
1:C:367:ASP:OD2	6:C:3005:FAD:N3	2.16	0.78
1:B:1176:HIS:NE2	7:B:2156:HOH:O	2.03	0.78
1:C:640:ASP:OD2	7:C:2083:HOH:O	2.02	0.78
1:A:1077:PRO:HG3	1:B:1027:GLN:HG3	1.65	0.78
6:B:3005:FAD:O2'	6:B:3005:FAD:C9	2.30	0.78
1:B:314:GLN:CD	7:B:2052:HOH:O	2.27	0.78
1:D:90:THR:O	7:D:2012:HOH:O	2.00	0.78
1:B:769:VAL:HG13	7:B:2115:HOH:O	1.83	0.78
1:C:1171:CYS:O	7:C:2136:HOH:O	2.00	0.78
1:D:216:LEU:CD1	1:D:216:LEU:H	1.96	0.77
1:D:308:THR:O	7:D:2057:HOH:O	2.01	0.77
1:B:1199:GLN:OE1	7:B:2159:HOH:O	2.02	0.77
1:C:1097:ASN:HD22	1:C:1137:TYR:H	1.33	0.77
1:B:704:GLN:H	1:B:704:GLN:HE21	1.30	0.77
1:B:1032:GLY:O	7:B:2141:HOH:O	2.02	0.76
1:D:95:ILE:O	7:D:2024:HOH:O	2.03	0.76
1:A:645:ARG:NH1	7:A:2108:HOH:O	2.04	0.76
1:A:964:PHE:O	7:A:2146:HOH:O	2.01	0.76
1:D:201:LEU:HD11	1:D:565:GLN:HG3	1.66	0.76
1:B:333:ILE:HG22	1:B:425:VAL:HG11	1.65	0.76
1:C:333:ILE:HG22	1:C:425:VAL:HG11	1.66	0.76
1:C:1103:MET:HA	1:C:1103:MET:HE2	1.67	0.76
1:B:900:ARG:NH1	1:B:902:ARG:HH22	1.84	0.76
1:C:213:THR:O	7:C:2033:HOH:O	2.04	0.76
1:B:1097:ASN:HD22	1:B:1137:TYR:H	1.34	0.76
1:A:333:ILE:HG22	1:A:425:VAL:HG11	1.67	0.75
1:C:983:TYR:O	7:C:2114:HOH:O	2.04	0.75
6:B:3005:FAD:H8A	6:B:3005:FAD:C5B	2.15	0.75
1:D:333:ILE:HG22	1:D:425:VAL:HG11	1.68	0.75
1:A:316:LYS:HG3	7:A:2060:HOH:O	1.86	0.75
1:A:1097:ASN:HD22	1:A:1137:TYR:H	1.35	0.75
1:A:1103:MET:HE2	1:A:1103:MET:HA	1.69	0.75
1:B:1248:LEU:HA	7:B:2158:HOH:O	1.86	0.75
1:D:1097:ASN:HD22	1:D:1137:TYR:H	1.35	0.75
1:C:101:ARG:NH1	7:C:2019:HOH:O	2.19	0.75
1:A:92:VAL:HA	1:A:126:MET:HE1	1.69	0.75
1:A:1027:GLN:HG3	1:B:1077:PRO:HG3	1.69	0.75
1:C:101:ARG:HD2	7:C:2019:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:900:ARG:NH1	1:D:902:ARG:HH22	1.85	0.74
1:D:655:GLU:OE2	7:D:2096:HOH:O	2.06	0.74
1:A:900:ARG:NH1	1:A:902:ARG:HH22	1.85	0.74
1:D:773:ASP:HB3	7:D:2111:HOH:O	1.87	0.74
1:C:1027:GLN:HG3	1:D:1077:PRO:HG3	1.69	0.74
1:B:445:MET:HG2	1:B:461:ILE:HG23	1.69	0.74
1:B:867:GLN:OE1	1:B:869:TYR:OH	2.02	0.74
1:A:31:LEU:CD2	1:A:45:TYR:HB3	2.18	0.74
1:D:655:GLU:CD	7:D:2096:HOH:O	2.30	0.74
1:D:655:GLU:HG3	7:D:2096:HOH:O	1.88	0.74
1:B:1312:GLU:HB3	1:B:1316:THR:HG21	1.69	0.74
1:D:1103:MET:HE2	1:D:1103:MET:HA	1.69	0.74
1:A:917:ARG:NH2	4:A:3003:MTE:HN8	1.86	0.74
1:B:909:ASN:ND2	7:B:2126:HOH:O	2.17	0.74
1:A:704:GLN:H	1:A:704:GLN:HE21	1.34	0.73
1:A:683:GLN:OE1	7:A:2120:HOH:O	2.06	0.73
1:B:92:VAL:HA	1:B:126:MET:HE1	1.70	0.73
1:B:251:ASP:OD2	7:B:2045:HOH:O	2.05	0.73
1:C:367:ASP:N	6:C:3005:FAD:O2	2.20	0.73
1:A:418:ARG:N	7:A:2057:HOH:O	2.20	0.73
1:A:445:MET:HG2	1:A:461:ILE:HG23	1.69	0.73
1:D:867:GLN:OE1	1:D:869:TYR:OH	2.03	0.73
1:A:1093:ARG:HH11	1:A:1093:ARG:HG3	1.54	0.73
1:B:528:LEU:HD12	1:B:552:ILE:HD11	1.70	0.73
1:D:826:ARG:HB2	1:D:827:PRO:HD2	1.71	0.73
1:A:363:LEU:N	7:A:2065:HOH:O	2.16	0.72
1:D:1093:ARG:HH11	1:D:1093:ARG:HG3	1.54	0.72
1:A:303:GLY:HA2	7:A:2057:HOH:O	1.89	0.72
1:A:358:HIS:HE2	1:A:366:SER:HG	1.33	0.72
1:C:445:MET:HG2	1:C:461:ILE:HG23	1.70	0.72
1:A:826:ARG:HB2	1:A:827:PRO:HD2	1.72	0.72
1:D:264:LEU:O	6:D:3005:FAD:H2B	1.89	0.72
1:D:1142:GLN:HG2	7:D:2140:HOH:O	1.88	0.72
1:C:92:VAL:HA	1:C:126:MET:HE1	1.70	0.72
1:C:31:LEU:CD2	1:C:45:TYR:HB3	2.19	0.72
1:C:506:ALA:HB1	1:C:512:GLU:CD	2.13	0.72
1:D:92:VAL:HA	1:D:126:MET:HE1	1.70	0.72
1:B:938:LYS:HZ1	1:B:1295:ILE:HD13	1.55	0.72
1:C:1256:LYS:NZ	7:C:2142:HOH:O	1.97	0.72
1:D:308:THR:HG21	6:D:3005:FAD:N6A	2.05	0.72
1:A:231:ASN:O	7:A:2043:HOH:O	2.08	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:927:VAL:HG23	7:C:2112:HOH:O	1.89	0.72
1:B:314:GLN:OE1	7:B:2052:HOH:O	2.07	0.72
1:B:358:HIS:HE2	1:B:366:SER:HG	1.34	0.72
1:B:1065:TYR:HB3	7:B:2141:HOH:O	1.90	0.72
1:A:130:THR:HG23	7:A:2015:HOH:O	1.90	0.71
1:A:1219:SER:OG	1:A:1223:VAL:HG12	1.90	0.71
1:C:826:ARG:HB2	1:C:827:PRO:HD2	1.71	0.71
6:D:3005:FAD:O4	7:D:2061:HOH:O	2.08	0.71
1:C:308:THR:HG21	6:C:3005:FAD:N6A	2.05	0.71
1:C:506:ALA:O	1:C:507:ALA:HB3	1.91	0.71
1:A:8:ASP:OD1	7:A:2002:HOH:O	2.07	0.71
1:A:340:GLN:HA	7:A:2062:HOH:O	1.90	0.71
1:B:337:LEU:HD23	1:B:371:ILE:HD11	1.72	0.71
1:C:923:GLN:O	7:C:2112:HOH:O	2.08	0.71
1:B:1103:MET:HE2	1:B:1103:MET:HA	1.72	0.71
1:D:269:THR:OG1	6:D:3005:FAD:O3'	1.81	0.71
1:A:1145:MET:N	7:A:2152:HOH:O	2.22	0.71
1:B:230:GLN:N	7:B:2039:HOH:O	2.24	0.71
1:D:445:MET:HG2	1:D:461:ILE:HG23	1.71	0.71
1:B:1161:GLY:HA3	1:B:1185:MET:HE2	1.71	0.70
1:C:269:THR:OG1	6:C:3005:FAD:H5'2	1.90	0.70
1:C:1161:GLY:HA3	1:C:1185:MET:HE2	1.73	0.70
1:A:1161:GLY:HA3	1:A:1185:MET:HE2	1.71	0.70
6:A:3005:FAD:O3B	7:A:2182:HOH:O	2.00	0.70
1:B:1093:ARG:HH11	1:B:1093:ARG:HG3	1.54	0.70
1:C:1093:ARG:HH11	1:C:1093:ARG:HG2	1.56	0.70
1:D:31:LEU:CD2	1:D:45:TYR:HB3	2.21	0.70
1:D:1161:GLY:HA3	1:D:1185:MET:HE2	1.72	0.70
1:A:213:THR:O	7:A:2039:HOH:O	2.10	0.70
1:D:1015:PRO:HA	1:D:1154:ILE:HG22	1.73	0.70
1:B:458:ASP:OD1	1:B:459:LEU:N	2.24	0.70
1:B:1087:GLY:N	4:B:3003:MTE:O1P	2.24	0.70
1:B:31:LEU:CD2	1:B:45:TYR:HB3	2.22	0.70
1:B:41:THR:OG1	7:B:2015:HOH:O	2.08	0.70
1:D:630:SER:N	7:D:2090:HOH:O	2.25	0.70
1:C:337:LEU:HD23	1:C:371:ILE:HD11	1.74	0.69
1:C:1015:PRO:HA	1:C:1154:ILE:HG22	1.73	0.69
1:B:1015:PRO:HA	1:B:1154:ILE:HG22	1.74	0.69
1:D:689:VAL:O	7:D:2102:HOH:O	2.08	0.69
1:A:337:LEU:HD23	1:A:371:ILE:HD11	1.73	0.69
1:B:636:LEU:N	7:B:2095:HOH:O	2.19	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:865:ASP:OD2	1:D:900:ARG:NH1	2.26	0.69
1:A:1015:PRO:HA	1:A:1154:ILE:HG22	1.73	0.69
1:C:683:GLN:OE1	7:C:2089:HOH:O	2.09	0.69
1:C:1093:ARG:HH11	1:C:1093:ARG:HG3	1.56	0.69
1:D:1205:VAL:HB	7:D:2030:HOH:O	1.91	0.69
1:A:490:LEU:HD12	1:A:527:TYR:CG	2.28	0.69
1:B:293:GLU:OE1	7:B:2050:HOH:O	2.11	0.69
1:B:967:THR:O	7:B:2131:HOH:O	2.10	0.69
1:C:1178:ASN:ND2	1:C:1239:ASP:O	2.25	0.69
1:D:216:LEU:H	1:D:216:LEU:HD12	1.55	0.69
1:A:573:GLN:N	7:A:2093:HOH:O	2.26	0.69
1:B:528:LEU:HD11	1:B:549:LEU:HD12	1.75	0.69
1:D:353:ALA:HB1	6:D:3005:FAD:H4'	1.75	0.69
1:D:636:LEU:N	7:D:2092:HOH:O	2.26	0.69
1:C:1219:SER:OG	1:C:1223:VAL:HG12	1.93	0.68
1:A:745:GLU:O	7:A:2034:HOH:O	2.10	0.68
1:B:1219:SER:OG	1:B:1223:VAL:HG12	1.92	0.68
1:A:569:ASP:OD1	7:A:2090:HOH:O	2.11	0.68
1:C:982:TYR:O	7:C:2114:HOH:O	2.11	0.68
1:D:358:HIS:HE2	1:D:366:SER:HG	1.38	0.68
1:A:626:SER:O	7:A:2105:HOH:O	2.12	0.68
1:B:739:VAL:HG11	1:B:930:THR:HG21	1.75	0.68
1:B:769:VAL:HG22	7:B:2115:HOH:O	1.93	0.68
1:A:865:ASP:OD2	1:A:900:ARG:NH1	2.27	0.68
1:B:490:LEU:HD12	1:B:527:TYR:CG	2.29	0.68
1:B:415:PHE:C	1:B:415:PHE:HD1	2.02	0.68
1:D:85:HIS:HA	7:D:2002:HOH:O	1.92	0.68
1:A:574:GLN:OE1	7:A:2094:HOH:O	2.10	0.68
1:A:948:GLU:C	7:A:2143:HOH:O	2.35	0.68
1:A:764:GLU:OE2	7:A:2130:HOH:O	2.12	0.68
1:C:703:VAL:HG13	1:C:704:GLN:NE2	2.09	0.67
1:A:254:GLU:OE1	7:A:2049:HOH:O	2.12	0.67
1:B:1178:ASN:ND2	1:B:1239:ASP:O	2.25	0.67
1:C:739:VAL:HG11	1:C:930:THR:HG21	1.76	0.67
1:B:1093:ARG:HH11	1:B:1093:ARG:HG2	1.56	0.67
1:A:408:GLU:O	7:A:2048:HOH:O	2.12	0.67
1:B:865:ASP:OD2	1:B:900:ARG:NH1	2.28	0.67
1:C:656:GLU:OE1	7:C:2087:HOH:O	2.11	0.67
1:B:230:GLN:O	7:B:2040:HOH:O	2.12	0.67
1:C:490:LEU:HD12	1:C:527:TYR:CG	2.30	0.67
1:D:752:GLN:HG2	1:D:813:LEU:CD1	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:VAL:O	7:B:2142:HOH:O	2.12	0.67
1:A:574:GLN:N	7:A:2093:HOH:O	2.27	0.67
1:B:41:THR:OG1	7:B:2014:HOH:O	1.86	0.67
1:D:1219:SER:OG	1:D:1223:VAL:HG12	1.94	0.67
1:D:557:PRO:O	7:D:2078:HOH:O	2.13	0.66
1:A:1093:ARG:HH11	1:A:1093:ARG:HG2	1.60	0.66
1:C:358:HIS:HE2	1:C:366:SER:HG	1.37	0.66
1:C:389:GLN:HA	7:C:2060:HOH:O	1.95	0.66
1:B:240:ARG:NH2	1:B:281:SER:HB2	2.10	0.66
1:C:1136:GLY:C	7:C:2119:HOH:O	2.37	0.66
1:D:1093:ARG:HH11	1:D:1093:ARG:HG2	1.59	0.66
1:A:490:LEU:C	1:A:490:LEU:HD23	2.20	0.66
1:A:752:GLN:HG2	1:A:813:LEU:CD1	2.24	0.66
1:B:875:THR:O	7:B:2124:HOH:O	2.13	0.66
1:B:1287:ARG:NH2	7:B:2162:HOH:O	2.27	0.66
1:A:1087:GLY:HA3	4:A:3003:MTE:O1P	1.96	0.66
1:C:505:MET:HB3	1:C:506:ALA:CA	2.26	0.66
1:D:15:ASN:ND2	7:D:2004:HOH:O	2.27	0.66
1:D:1178:ASN:ND2	1:D:1239:ASP:O	2.24	0.66
1:B:547:GLN:OE1	1:B:547:GLN:N	2.28	0.66
1:A:108:ARG:O	7:A:2025:HOH:O	2.12	0.66
1:A:809:LYS:HE3	1:A:841:THR:O	1.96	0.66
1:A:1178:ASN:ND2	1:A:1239:ASP:O	2.28	0.66
1:B:826:ARG:HB2	1:B:827:PRO:HD2	1.78	0.66
1:B:710:GLU:HG3	1:B:712:PHE:HE2	1.61	0.66
1:D:739:VAL:HG11	1:D:930:THR:HG21	1.75	0.66
1:B:490:LEU:C	1:B:490:LEU:HD23	2.21	0.65
1:B:809:LYS:HE3	1:B:841:THR:O	1.96	0.65
1:C:752:GLN:HG2	1:C:813:LEU:CD1	2.27	0.65
1:C:332:GLN:OE1	7:C:2054:HOH:O	2.14	0.65
1:A:372:LEU:O	7:A:2067:HOH:O	2.14	0.65
1:A:710:GLU:HG3	1:A:712:PHE:HE2	1.61	0.65
1:B:267:GLY:HA3	6:B:3005:FAD:O2P	1.96	0.65
1:C:741:LEU:HD11	1:C:926:PHE:HD2	1.61	0.65
1:D:202:TYR:OH	7:D:2034:HOH:O	2.15	0.65
1:B:752:GLN:HG2	1:B:813:LEU:CD1	2.25	0.65
1:A:343:THR:O	7:A:2063:HOH:O	2.15	0.65
1:A:741:LEU:HD11	1:A:926:PHE:HD2	1.62	0.65
1:A:114:GLY:HA2	1:A:159:PRO:HB2	1.79	0.65
1:C:490:LEU:HD23	1:C:490:LEU:C	2.21	0.65
1:A:339:LYS:O	7:A:2062:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1076:VAL:O	7:D:2136:HOH:O	2.15	0.65
1:C:376:ASN:OD1	7:C:2059:HOH:O	2.15	0.64
1:D:415:PHE:C	1:D:415:PHE:CD1	2.74	0.64
1:D:741:LEU:HA	1:D:1300:SER:HB3	1.80	0.64
1:C:471:ILE:HD12	1:C:504:LEU:HD12	1.79	0.64
1:D:8:ASP:O	7:D:2001:HOH:O	2.14	0.64
1:D:892:ASN:O	1:D:1009:LYS:HE3	1.97	0.64
1:C:884:GLU:OE1	1:C:1147:TRP:NE1	2.31	0.64
1:B:741:LEU:HD11	1:B:926:PHE:HD2	1.63	0.64
1:C:590:ILE:O	1:C:594:THR:HG23	1.98	0.64
1:B:353:ALA:HA	6:B:3005:FAD:O2P	1.97	0.64
1:B:493:ALA:O	1:B:497:ILE:HG12	1.98	0.64
1:B:890:LEU:O	1:B:928:THR:HG21	1.98	0.64
1:C:710:GLU:HG3	1:C:712:PHE:HE2	1.62	0.64
1:B:1238:THR:OG1	7:B:2062:HOH:O	2.13	0.64
1:A:739:VAL:HG11	1:A:930:THR:HG21	1.80	0.64
1:A:987:LYS:CE	7:A:2150:HOH:O	2.46	0.64
1:C:415:PHE:CD1	1:C:415:PHE:C	2.75	0.64
1:B:387:ILE:HD12	1:B:387:ILE:H	1.62	0.64
1:D:58:MET:HB3	7:D:2012:HOH:O	1.98	0.64
1:A:387:ILE:HD12	1:A:387:ILE:H	1.63	0.63
1:B:25:ASP:O	1:B:28:VAL:HG13	1.98	0.63
1:D:710:GLU:HG3	1:D:712:PHE:HE2	1.62	0.63
1:B:415:PHE:C	1:B:415:PHE:CD1	2.74	0.63
1:A:548:LYS:N	7:A:2086:HOH:O	2.31	0.63
1:B:59:ILE:HD11	1:B:72:PHE:CE2	2.34	0.63
1:B:892:ASN:O	1:B:1009:LYS:HE3	1.98	0.63
1:C:667:VAL:HG22	1:C:667:VAL:O	1.98	0.63
1:D:809:LYS:HE3	1:D:841:THR:O	1.97	0.63
1:C:387:ILE:HD12	1:C:387:ILE:H	1.64	0.63
1:D:15:ASN:CG	7:D:2004:HOH:O	2.42	0.63
1:A:892:ASN:O	1:A:1009:LYS:HE3	1.98	0.63
1:C:809:LYS:HE3	1:C:841:THR:O	1.98	0.63
1:D:776:PHE:CE1	1:D:780:MET:HE3	2.34	0.63
1:B:63:ASP:N	7:B:2018:HOH:O	2.32	0.63
1:C:776:PHE:CE1	1:C:780:MET:HE3	2.34	0.63
1:C:530:VAL:O	1:C:534:LEU:HG	1.99	0.62
1:D:59:ILE:HD11	1:D:72:PHE:CE2	2.33	0.62
1:C:506:ALA:HB1	1:C:512:GLU:CG	2.30	0.62
1:B:310:LEU:HD23	7:B:2052:HOH:O	1.98	0.62
1:B:379:LEU:HD12	7:B:2055:HOH:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:GLY:HA2	1:B:159:PRO:HB2	1.81	0.62
1:D:59:ILE:HG13	1:D:72:PHE:CZ	2.33	0.62
1:D:72:PHE:N	7:D:2013:HOH:O	2.33	0.62
1:B:703:VAL:HG13	1:B:704:GLN:NE2	2.15	0.62
1:C:890:LEU:O	1:C:928:THR:HG21	1.99	0.62
1:D:782:ALA:HB1	1:D:787:ILE:O	2.00	0.62
1:A:741:LEU:HA	1:A:1300:SER:HB3	1.82	0.62
1:A:761:GLU:HG3	1:B:591:LYS:CD	2.30	0.62
1:B:156:GLY:O	1:B:1240:ILE:HD12	2.00	0.62
1:B:435:GLN:CG	7:B:2029:HOH:O	2.47	0.62
1:C:334:TYR:HE1	1:C:416:VAL:HG22	1.65	0.62
1:B:310:LEU:HA	7:B:2052:HOH:O	1.99	0.62
1:B:552:ILE:HG13	1:B:553:LEU:HD23	1.82	0.62
1:B:704:GLN:H	1:B:704:GLN:NE2	1.98	0.62
1:D:25:ASP:O	1:D:28:VAL:HG13	2.00	0.62
1:A:890:LEU:O	1:A:928:THR:HG21	2.00	0.61
1:B:1154:ILE:HD12	1:B:1155:PHE:CZ	2.35	0.61
1:B:1185:MET:O	7:B:2158:HOH:O	2.16	0.61
1:D:890:LEU:O	1:D:928:THR:HG21	1.99	0.61
1:A:692:VAL:N	7:A:2105:HOH:O	2.32	0.61
1:B:59:ILE:HG13	1:B:72:PHE:CZ	2.35	0.61
1:D:216:LEU:HD12	1:D:216:LEU:N	2.15	0.61
1:B:344:LEU:HD12	1:B:344:LEU:C	2.25	0.61
1:B:471:ILE:HD12	1:B:504:LEU:HD12	1.81	0.61
1:B:712:PHE:CD1	1:B:904:ARG:HD3	2.36	0.61
1:C:892:ASN:O	1:C:1009:LYS:HE3	2.00	0.61
1:D:590:ILE:O	1:D:594:THR:HG23	2.00	0.61
1:A:590:ILE:O	1:A:594:THR:HG23	1.99	0.61
1:B:900:ARG:HH11	1:B:902:ARG:HH22	1.47	0.61
1:D:207:PHE:HB3	7:D:2026:HOH:O	2.00	0.61
1:A:916:PHE:HZ	7:A:2034:HOH:O	1.82	0.61
1:B:47:CYS:SG	1:B:48:GLY:N	2.73	0.61
1:B:357:GLY:HA3	6:B:3005:FAD:O1P	2.01	0.61
1:B:776:PHE:CE1	1:B:780:MET:HE3	2.36	0.61
1:C:719:LEU:HD11	1:C:888:LEU:HD23	1.83	0.61
1:D:344:LEU:C	1:D:344:LEU:HD12	2.26	0.61
1:C:741:LEU:HA	1:C:1300:SER:HB3	1.83	0.61
1:D:1087:GLY:HA3	4:D:3003:MTE:O1P	2.00	0.61
1:D:1154:ILE:HD12	1:D:1155:PHE:CZ	2.36	0.61
1:A:667:VAL:O	1:A:667:VAL:HG22	2.00	0.61
1:A:25:ASP:O	1:A:28:VAL:HG13	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:LEU:N	7:A:2086:HOH:O	1.99	0.61
1:C:114:GLY:HA2	1:C:159:PRO:HB2	1.83	0.61
1:A:59:ILE:HD11	1:A:72:PHE:CE2	2.36	0.60
1:A:645:ARG:NH2	7:A:2110:HOH:O	2.33	0.60
1:A:967:THR:N	7:A:2147:HOH:O	2.33	0.60
1:B:148:GLY:HA3	7:B:2029:HOH:O	2.00	0.60
1:D:334:TYR:HE1	1:D:416:VAL:HG22	1.66	0.60
1:A:334:TYR:HE1	1:A:416:VAL:HG22	1.66	0.60
1:C:25:ASP:O	1:C:28:VAL:HG13	2.01	0.60
1:C:270:TYR:HB3	6:C:3005:FAD:O1A	2.01	0.60
1:C:344:LEU:C	1:C:344:LEU:HD12	2.27	0.60
1:C:415:PHE:C	1:C:415:PHE:HD1	2.10	0.60
1:C:753:SER:HB3	1:C:831:ILE:HD13	1.83	0.60
1:D:357:GLY:HA2	6:D:3005:FAD:H51A	1.83	0.60
1:A:884:GLU:OE1	1:A:1147:TRP:NE1	2.34	0.60
1:B:652:GLY:HA3	1:B:656:GLU:O	2.02	0.60
1:B:667:VAL:HG22	1:B:667:VAL:O	2.00	0.60
1:D:727:ALA:HB2	1:D:898:ASN:ND2	2.16	0.60
1:A:712:PHE:CD1	1:A:904:ARG:HD3	2.35	0.60
1:A:887:LEU:HD22	1:A:901:VAL:HG22	1.84	0.60
7:A:2154:HOH:O	1:B:1074:VAL:O	2.16	0.60
1:C:199:THR:O	7:C:2027:HOH:O	2.16	0.60
1:B:590:ILE:O	1:B:594:THR:HG23	2.01	0.60
1:B:741:LEU:HA	1:B:1300:SER:HB3	1.83	0.60
1:D:956:ASP:OD1	1:D:957:ARG:N	2.32	0.60
1:A:552:ILE:HG13	1:A:553:LEU:HD23	1.83	0.60
1:C:59:ILE:HD11	1:C:72:PHE:CE2	2.37	0.60
1:C:59:ILE:HG13	1:C:72:PHE:CZ	2.37	0.60
1:C:367:ASP:HB2	6:C:3005:FAD:O2	2.02	0.60
1:C:614:VAL:HG12	1:C:673:ALA:HB2	1.83	0.60
1:C:652:GLY:HA3	1:C:656:GLU:O	2.01	0.60
1:C:256:LYS:HE3	1:C:407:PRO:O	2.02	0.59
1:A:156:GLY:O	1:A:1240:ILE:HD12	2.01	0.59
1:A:591:LYS:CD	1:B:761:GLU:HG3	2.32	0.59
1:A:900:ARG:HH11	1:A:902:ARG:HH22	1.48	0.59
1:B:310:LEU:CD2	7:B:2052:HOH:O	2.48	0.59
1:B:334:TYR:HE1	1:B:416:VAL:HG22	1.65	0.59
1:A:59:ILE:HG13	1:A:72:PHE:CZ	2.37	0.59
1:A:257:MET:HG2	1:A:384:THR:HG21	1.84	0.59
1:C:50:GLY:HA2	3:C:3002:FES:S2	2.43	0.59
1:C:381:VAL:N	7:C:2060:HOH:O	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ASP:HB3	1:B:28:VAL:CG1	2.32	0.59
1:B:614:VAL:HG12	1:B:673:ALA:HB2	1.84	0.59
1:C:741:LEU:HD11	1:C:926:PHE:CD2	2.37	0.59
1:D:712:PHE:CD1	1:D:904:ARG:HD3	2.37	0.59
1:D:114:GLY:HA2	1:D:159:PRO:HB2	1.83	0.59
1:A:471:ILE:HD12	1:A:504:LEU:HD12	1.82	0.59
1:C:788:PRO:HG2	1:C:791:ARG:NH1	2.18	0.59
1:D:587:GLN:HG3	7:D:2085:HOH:O	2.03	0.59
1:C:578:ASP:C	1:C:578:ASP:OD1	2.45	0.59
1:D:655:GLU:CG	7:D:2096:HOH:O	2.45	0.59
1:A:503:LEU:O	7:A:2077:HOH:O	2.17	0.59
1:A:703:VAL:HG13	1:A:704:GLN:NE2	2.18	0.59
1:C:251:ASP:CG	7:C:2043:HOH:O	2.44	0.59
1:C:704:GLN:H	1:C:704:GLN:NE2	1.99	0.59
1:D:652:GLY:HA3	1:D:656:GLU:O	2.02	0.59
1:D:900:ARG:HH11	1:D:902:ARG:HH22	1.48	0.59
1:A:741:LEU:HD11	1:A:926:PHE:CD2	2.38	0.58
1:A:776:PHE:CE1	1:A:780:MET:HE3	2.38	0.58
1:A:1206:GLN:HG3	7:A:2033:HOH:O	2.03	0.58
1:B:1045:GLN:OE1	1:B:1045:GLN:N	2.30	0.58
1:C:47:CYS:SG	1:C:48:GLY:N	2.75	0.58
1:A:25:ASP:HB3	1:A:28:VAL:CG1	2.33	0.58
1:A:344:LEU:C	1:A:344:LEU:HD12	2.28	0.58
1:C:1085:SER:HA	4:C:3003:MTE:O2P	2.03	0.58
1:D:480:LEU:HG	7:D:2074:HOH:O	2.03	0.58
1:B:264:LEU:O	6:B:3005:FAD:H2B	2.03	0.58
1:C:703:VAL:HG12	1:C:1334:VAL:O	2.03	0.58
1:D:667:VAL:O	1:D:667:VAL:HG22	2.02	0.58
1:D:415:PHE:C	1:D:415:PHE:HD1	2.11	0.58
1:D:917:ARG:NH2	4:D:3003:MTE:HN8	2.01	0.58
1:A:1157:TYR:CE1	1:A:1262:LYS:HG3	2.38	0.58
1:A:727:ALA:HB2	1:A:898:ASN:ND2	2.18	0.58
1:B:727:ALA:HB2	1:B:898:ASN:ND2	2.18	0.58
1:B:1157:TYR:CE1	1:B:1262:LYS:HG3	2.39	0.58
1:A:956:ASP:OD1	1:A:957:ARG:N	2.35	0.58
1:C:1157:TYR:CE1	1:C:1262:LYS:HG3	2.39	0.58
1:A:201:LEU:CD1	1:A:565:GLN:HG3	2.30	0.58
1:A:358:HIS:HB2	6:A:3005:FAD:O4'	2.04	0.58
1:A:704:GLN:H	1:A:704:GLN:NE2	2.02	0.57
1:B:703:VAL:HG12	1:B:1334:VAL:O	2.03	0.57
1:B:782:ALA:HB1	1:B:787:ILE:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:887:LEU:HD22	1:C:901:VAL:HG22	1.85	0.57
1:D:719:LEU:HD11	1:D:888:LEU:HD23	1.86	0.57
1:A:356:GLY:N	7:A:2058:HOH:O	2.36	0.57
1:A:667:VAL:HG11	1:A:1222:GLY:O	2.03	0.57
1:D:25:ASP:HB3	1:D:28:VAL:CG1	2.33	0.57
1:B:1084:ALA:O	1:B:1086:THR:HG22	2.02	0.57
6:B:3005:FAD:H52A	6:B:3005:FAD:C8A	2.28	0.57
1:C:761:GLU:HG3	1:D:591:LYS:CD	2.34	0.57
1:A:685:ALA:HA	1:A:688:LYS:HD2	1.87	0.57
1:A:753:SER:HB3	1:A:831:ILE:HD13	1.86	0.57
1:B:719:LEU:HD11	1:B:888:LEU:HD23	1.87	0.57
1:A:703:VAL:HG12	1:A:1334:VAL:O	2.04	0.57
1:A:788:PRO:HG2	1:A:791:ARG:NH1	2.20	0.57
1:B:741:LEU:HD11	1:B:926:PHE:CD2	2.39	0.57
1:C:1045:GLN:OE1	1:C:1045:GLN:N	2.33	0.57
1:D:578:ASP:OD1	1:D:578:ASP:C	2.46	0.57
1:A:719:LEU:HD11	1:A:888:LEU:HD23	1.86	0.57
1:A:1154:ILE:HD12	1:A:1155:PHE:CZ	2.39	0.57
1:C:156:GLY:O	1:C:1240:ILE:HD12	2.05	0.57
1:A:652:GLY:HA3	1:A:656:GLU:O	2.04	0.57
1:A:916:PHE:O	1:A:917:ARG:C	2.48	0.57
1:B:770:SER:C	7:B:2115:HOH:O	2.39	0.57
1:C:387:ILE:HD12	1:C:387:ILE:N	2.20	0.57
1:C:507:ALA:HB1	1:C:508:PRO:HD2	1.86	0.57
1:C:1154:ILE:HD12	1:C:1155:PHE:CZ	2.39	0.57
1:D:147:LEU:O	1:D:149:GLY:N	2.38	0.57
1:A:256:LYS:HE3	1:A:407:PRO:O	2.05	0.57
1:A:674:VAL:CG1	1:A:686:ALA:HB2	2.34	0.57
1:D:798:ARG:HH11	1:D:798:ARG:HG2	1.70	0.57
1:A:338:LEU:HD21	7:A:2060:HOH:O	2.04	0.57
1:A:1093:ARG:CG	1:A:1093:ARG:NH1	2.57	0.57
1:C:1077:PRO:CG	1:D:1027:GLN:HG3	2.35	0.57
1:A:376:ASN:N	7:A:2067:HOH:O	2.37	0.56
1:B:887:LEU:HD22	1:B:901:VAL:HG22	1.87	0.56
1:A:1085:SER:HA	4:A:3003:MTE:O3P	2.04	0.56
1:B:387:ILE:HD12	1:B:387:ILE:N	2.20	0.56
1:D:240:ARG:NH2	1:D:281:SER:HB2	2.20	0.56
1:D:703:VAL:HG12	1:D:1334:VAL:O	2.04	0.56
1:D:1157:TYR:CE1	1:D:1262:LYS:HG3	2.39	0.56
1:A:50:GLY:HA2	3:A:3002:FES:S2	2.45	0.56
1:A:591:LYS:HD3	1:B:761:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ALA:HB1	1:A:787:ILE:O	2.05	0.56
1:B:580:ILE:CG1	1:B:1057:ARG:HG3	2.35	0.56
1:C:667:VAL:HG11	1:C:1222:GLY:O	2.05	0.56
1:D:90:THR:HB	7:D:2012:HOH:O	2.04	0.56
1:D:580:ILE:CG1	1:D:1057:ARG:HG3	2.36	0.56
1:D:753:SER:HB3	1:D:831:ILE:HD13	1.87	0.56
1:B:450:LYS:O	1:B:451:GLU:C	2.49	0.56
1:B:545:ILE:HG23	1:B:545:ILE:O	2.04	0.56
1:B:625:ILE:HG21	1:C:692:VAL:HG21	1.87	0.56
1:A:723:ASN:OD1	1:A:725:GLU:HG2	2.06	0.56
1:B:147:LEU:O	1:B:149:GLY:N	2.39	0.56
1:C:25:ASP:HB3	1:C:28:VAL:CG1	2.34	0.56
1:D:1206:GLN:N	7:D:2030:HOH:O	2.38	0.56
1:B:578:ASP:OD1	1:B:578:ASP:C	2.46	0.56
1:B:667:VAL:HG11	1:B:1222:GLY:O	2.06	0.56
1:D:156:GLY:O	1:D:1240:ILE:HD12	2.06	0.56
1:D:50:GLY:HA2	3:D:3002:FES:S2	2.45	0.56
1:D:256:LYS:HE3	1:D:407:PRO:O	2.05	0.56
1:A:968:ASN:N	7:A:2148:HOH:O	2.29	0.56
1:A:47:CYS:SG	1:A:48:GLY:N	2.74	0.56
1:B:788:PRO:HG2	1:B:791:ARG:NH1	2.21	0.56
1:B:868:LEU:HD12	1:B:887:LEU:HD23	1.88	0.56
1:B:422:TRP:CD1	1:B:451:GLU:HA	2.41	0.56
1:C:782:ALA:HB1	1:C:787:ILE:O	2.06	0.56
1:A:951:MET:HB2	7:A:2143:HOH:O	2.06	0.55
1:B:32:PHE:CE1	1:B:36:LYS:HG3	2.41	0.55
1:C:434:GLN:N	7:C:2064:HOH:O	2.32	0.55
1:C:764:GLU:OE2	7:C:2100:HOH:O	2.18	0.55
1:A:363:LEU:HG	7:A:2065:HOH:O	2.06	0.55
1:D:887:LEU:HD22	1:D:901:VAL:HG22	1.87	0.55
1:D:921:PHE:N	1:D:922:PRO:HD2	2.21	0.55
1:A:387:ILE:HD12	1:A:387:ILE:N	2.20	0.55
1:A:578:ASP:C	1:A:578:ASP:OD1	2.49	0.55
1:B:771:SER:CB	7:B:2115:HOH:O	2.54	0.55
1:B:230:GLN:N	7:B:2040:HOH:O	2.39	0.55
1:D:614:VAL:HG12	1:D:673:ALA:HB2	1.89	0.55
1:D:667:VAL:HG11	1:D:1222:GLY:O	2.07	0.55
1:D:1084:ALA:O	1:D:1086:THR:HG22	2.06	0.55
1:B:1110:ILE:O	1:B:1110:ILE:HG13	2.06	0.55
1:D:609:GLU:HA	1:D:827:PRO:HG2	1.89	0.55
1:C:27:GLU:HG3	7:C:2004:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1047:ILE:HG23	7:C:2130:HOH:O	2.07	0.55
1:C:103:HIS:CE1	1:C:105:VAL:HG23	2.42	0.55
1:C:415:PHE:HD1	1:C:416:VAL:N	2.05	0.55
1:C:609:GLU:HA	1:C:827:PRO:HG2	1.89	0.55
1:A:667:VAL:HG12	7:A:2117:HOH:O	2.06	0.55
1:B:344:LEU:HD13	6:B:3005:FAD:C10	2.37	0.55
1:B:956:ASP:OD1	1:B:957:ARG:N	2.33	0.55
1:C:591:LYS:CD	1:D:761:GLU:HG3	2.36	0.55
1:B:685:ALA:HA	1:B:688:LYS:HD2	1.89	0.55
1:D:92:VAL:HA	1:D:126:MET:CE	2.37	0.55
1:D:677:ASP:HB3	7:D:2093:HOH:O	2.05	0.55
1:B:154:CYS:O	1:B:1202:GLY:HA3	2.07	0.55
1:B:1093:ARG:CG	1:B:1093:ARG:NH1	2.55	0.55
1:C:358:HIS:HA	6:C:3005:FAD:O4'	2.07	0.55
1:C:299:ASN:ND2	7:C:2051:HOH:O	2.40	0.54
1:C:710:GLU:HG3	1:C:712:PHE:CE2	2.42	0.54
1:C:969:LEU:HB2	1:C:1160:PHE:CD1	2.41	0.54
1:D:788:PRO:HG2	1:D:791:ARG:NH1	2.22	0.54
1:A:710:GLU:HG3	1:A:712:PHE:CE2	2.41	0.54
1:A:921:PHE:N	1:A:922:PRO:HD2	2.22	0.54
1:A:1023:ALA:HB3	1:A:1076:VAL:HG13	1.89	0.54
1:C:713:ILE:HG13	1:C:907:LYS:CB	2.38	0.54
1:C:770:SER:O	1:C:806:LYS:HD3	2.07	0.54
1:C:868:LEU:HD12	1:C:887:LEU:HD23	1.90	0.54
1:C:1137:TYR:CD1	1:D:1131:SER:HB2	2.42	0.54
1:A:614:VAL:HG12	1:A:673:ALA:HB2	1.89	0.54
1:A:713:ILE:CG1	1:A:907:LYS:HB3	2.31	0.54
1:C:201:LEU:CD1	1:C:565:GLN:HG3	2.36	0.54
1:D:756:VAL:O	1:D:827:PRO:HA	2.07	0.54
1:A:868:LEU:HD12	1:A:887:LEU:HD23	1.90	0.54
1:A:1220:PRO:HA	1:A:1332:ILE:HD13	1.90	0.54
1:C:776:PHE:CZ	1:C:780:MET:HE3	2.42	0.54
1:A:917:ARG:CZ	1:A:1203:ALA:HB2	2.38	0.54
1:C:505:MET:CG	1:C:506:ALA:HA	2.37	0.54
1:C:916:PHE:O	1:C:917:ARG:C	2.49	0.54
1:C:921:PHE:N	1:C:922:PRO:HD2	2.23	0.54
1:C:1311:CYS:HB2	7:C:2136:HOH:O	2.07	0.54
1:D:1045:GLN:OE1	1:D:1045:GLN:N	2.33	0.54
1:A:383:SER:HB3	1:A:409:GLN:HB3	1.89	0.54
1:A:571:ASP:CB	7:A:2093:HOH:O	2.56	0.54
1:A:1196:ASP:HB3	1:A:1264:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ILE:HD11	1:B:416:VAL:HG23	1.90	0.54
1:B:884:GLU:OE1	1:B:1147:TRP:NE1	2.40	0.54
1:C:1111:LYS:O	1:C:1114:PRO:HD3	2.08	0.54
1:D:647:VAL:HG23	1:D:647:VAL:O	2.06	0.54
1:C:580:ILE:CG1	1:C:1057:ARG:HG3	2.38	0.54
1:D:333:ILE:HD11	1:D:416:VAL:HG23	1.89	0.54
1:D:674:VAL:CG1	1:D:686:ALA:HB2	2.37	0.54
1:A:987:LYS:NZ	7:A:2150:HOH:O	2.19	0.54
1:B:68:ARG:O	7:B:2018:HOH:O	2.19	0.54
1:A:1314:GLN:CD	1:A:1314:GLN:H	2.15	0.54
1:B:763:LYS:NZ	7:B:2114:HOH:O	2.39	0.54
1:C:360:ILE:HG13	6:C:3005:FAD:N3A	2.23	0.54
1:D:685:ALA:HA	1:D:688:LYS:HD2	1.89	0.54
1:C:1110:ILE:O	1:C:1110:ILE:HG13	2.07	0.54
1:D:1110:ILE:O	1:D:1110:ILE:HG13	2.07	0.54
1:A:133:ARG:NH2	1:D:213:THR:HG21	2.22	0.53
1:C:307:GLY:HA2	1:C:413:SER:HB3	1.90	0.53
1:D:383:SER:HB3	1:D:409:GLN:HB3	1.90	0.53
1:D:1067:HIS:ND1	7:D:2134:HOH:O	2.28	0.53
1:B:387:ILE:HG22	1:B:388:GLN:N	2.23	0.53
1:C:917:ARG:NH2	4:C:3003:MTE:HN8	2.06	0.53
1:C:917:ARG:CZ	1:C:1203:ALA:HB2	2.38	0.53
1:A:1137:TYR:CD1	1:B:1131:SER:HB2	2.43	0.53
1:B:753:SER:HB3	1:B:831:ILE:HD13	1.90	0.53
1:B:945:LYS:O	1:B:949:LEU:HG	2.08	0.53
1:C:383:SER:HB3	1:C:409:GLN:HB3	1.90	0.53
1:D:33:TYR:O	1:D:37:VAL:HG12	2.09	0.53
1:A:154:CYS:O	1:A:1202:GLY:HA3	2.09	0.53
1:A:387:ILE:HG22	1:A:388:GLN:N	2.22	0.53
1:A:1025:LEU:HD13	1:A:1135:THR:HG22	1.91	0.53
1:B:710:GLU:HG3	1:B:712:PHE:CE2	2.42	0.53
1:D:358:HIS:NE2	1:D:366:SER:OG	2.33	0.53
1:D:1220:PRO:HA	1:D:1332:ILE:HD13	1.90	0.53
1:A:92:VAL:HA	1:A:126:MET:CE	2.38	0.53
1:A:609:GLU:HA	1:A:827:PRO:HG2	1.90	0.53
1:B:647:VAL:O	1:B:647:VAL:HG23	2.07	0.53
1:C:333:ILE:HD11	1:C:416:VAL:HG23	1.90	0.53
1:C:1087:GLY:HA3	4:C:3003:MTE:O3P	2.09	0.53
1:C:1317:ASN:O	1:C:1318:LEU:HD23	2.08	0.53
1:D:868:LEU:HD12	1:D:887:LEU:HD23	1.90	0.53
1:D:884:GLU:OE1	1:D:1147:TRP:NE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1111:LYS:O	1:A:1114:PRO:HD3	2.07	0.53
1:B:1220:PRO:HA	1:B:1332:ILE:HD13	1.90	0.53
1:D:15:ASN:OD1	7:D:2004:HOH:O	2.19	0.53
1:A:580:ILE:CG1	1:A:1057:ARG:HG3	2.39	0.53
1:A:1018:PHE:O	1:A:1021:GLN:HG2	2.09	0.53
1:B:201:LEU:CD1	1:B:565:GLN:HG3	2.35	0.53
1:B:969:LEU:HB2	1:B:1160:PHE:CD1	2.43	0.53
1:C:303:GLY:HA3	1:C:415:PHE:CE1	2.44	0.53
1:C:1009:LYS:HD3	1:C:1158:PHE:CD2	2.44	0.53
1:C:337:LEU:HA	1:C:371:ILE:HD11	1.91	0.53
1:D:710:GLU:HG3	1:D:712:PHE:CE2	2.42	0.53
1:A:917:ARG:CZ	4:A:3003:MTE:HN8	2.22	0.53
1:B:900:ARG:HH11	1:B:902:ARG:NH2	2.07	0.53
1:B:1111:LYS:O	1:B:1114:PRO:HD3	2.09	0.53
1:C:265:VAL:HG13	1:C:265:VAL:O	2.08	0.53
1:C:578:ASP:OD2	1:C:1057:ARG:NH1	2.42	0.53
1:C:674:VAL:CG1	1:C:686:ALA:HB2	2.38	0.53
1:C:1084:ALA:O	1:C:1086:THR:HG22	2.09	0.53
1:D:945:LYS:O	1:D:949:LEU:HG	2.09	0.53
1:A:1093:ARG:HG3	1:A:1093:ARG:NH1	2.23	0.53
1:A:546:SER:CB	7:A:2086:HOH:O	2.57	0.52
1:A:761:GLU:OE2	1:B:798:ARG:NH2	2.40	0.52
1:B:921:PHE:N	1:B:922:PRO:HD2	2.24	0.52
1:C:92:VAL:HA	1:C:126:MET:CE	2.39	0.52
1:C:685:ALA:HA	1:C:688:LYS:HD2	1.91	0.52
1:D:32:PHE:CE1	1:D:36:LYS:HG3	2.45	0.52
1:D:1196:ASP:HB3	1:D:1264:LEU:HD12	1.91	0.52
1:A:337:LEU:HA	1:A:371:ILE:HD11	1.91	0.52
1:A:377:CYS:SG	1:A:416:VAL:HB	2.50	0.52
1:B:472:SER:C	1:B:474:ASP:H	2.16	0.52
1:D:103:HIS:CE1	1:D:105:VAL:HG23	2.44	0.52
1:A:606:LEU:HD23	1:B:606:LEU:HD23	1.91	0.52
1:A:969:LEU:HB2	1:A:1160:PHE:CD1	2.45	0.52
1:B:383:SER:HB3	1:B:409:GLN:HB3	1.91	0.52
1:D:264:LEU:HD13	1:D:286:ILE:HB	1.92	0.52
1:D:741:LEU:HA	1:D:1300:SER:CB	2.40	0.52
1:A:333:ILE:HD11	1:A:416:VAL:HG23	1.90	0.52
1:B:33:TYR:HA	1:B:37:VAL:HG12	1.91	0.52
1:B:1023:ALA:HB3	1:B:1076:VAL:HG13	1.91	0.52
1:C:483:ARG:NH2	1:C:489:MET:HA	2.25	0.52
1:D:270:TYR:HB3	6:D:3005:FAD:O1A	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:916:PHE:O	1:D:917:ARG:C	2.52	0.52
1:A:761:GLU:HG3	1:B:591:LYS:HD3	1.92	0.52
1:A:808:SER:HB3	7:A:2136:HOH:O	2.08	0.52
1:B:75:THR:OG1	7:B:2020:HOH:O	2.03	0.52
1:B:644:ALA:HB2	7:B:2097:HOH:O	2.08	0.52
1:B:1154:ILE:O	7:B:2154:HOH:O	2.18	0.52
1:A:66:SER:O	1:A:67:LYS:HB2	2.10	0.52
1:A:371:ILE:HA	1:A:374:ILE:HG22	1.92	0.52
1:A:761:GLU:HG3	1:B:591:LYS:HD2	1.91	0.52
1:A:1084:ALA:O	1:A:1086:THR:HG22	2.09	0.52
1:C:1136:GLY:O	7:C:2119:HOH:O	2.19	0.52
1:B:756:VAL:O	1:B:827:PRO:HA	2.10	0.52
1:B:776:PHE:CZ	1:B:780:MET:HE3	2.45	0.52
1:B:917:ARG:CZ	1:B:1203:ALA:HB2	2.40	0.52
1:C:63:ASP:O	1:C:67:LYS:N	2.40	0.52
1:C:467:GLY:HA3	1:C:471:ILE:CG2	2.40	0.52
1:D:297:VAL:HG13	1:D:297:VAL:O	2.10	0.52
1:D:514:TYR:CZ	1:D:518:LEU:HD11	2.45	0.52
1:A:483:ARG:NH2	1:A:489:MET:HA	2.25	0.52
1:A:676:ALA:HB3	1:A:682:ALA:HB2	1.92	0.52
1:A:764:GLU:CD	7:A:2130:HOH:O	2.53	0.52
1:A:900:ARG:HH11	1:A:902:ARG:NH2	2.08	0.52
1:B:674:VAL:CG1	1:B:686:ALA:HB2	2.40	0.52
1:B:984:ASN:O	1:B:987:LYS:HB2	2.09	0.52
1:C:33:TYR:HA	1:C:37:VAL:HG12	1.92	0.52
1:C:371:ILE:HA	1:C:374:ILE:HG22	1.92	0.52
1:C:756:VAL:O	1:C:827:PRO:HA	2.09	0.52
1:C:793:ASN:HB3	1:C:1074:VAL:CG2	2.40	0.52
1:C:1000:LYS:HE2	1:C:1286:ALA:HA	1.92	0.52
1:C:1043:LEU:HG	1:C:1045:GLN:HE22	1.75	0.52
1:D:243:TRP:HZ2	7:D:2051:HOH:O	1.93	0.52
1:D:507:ALA:HB1	1:D:508:PRO:HD2	1.91	0.52
1:D:1101:ILE:O	1:D:1105:ARG:HG3	2.09	0.52
1:A:1077:PRO:HD3	1:B:1027:GLN:OE1	2.10	0.52
1:B:337:LEU:HA	1:B:371:ILE:HD11	1.92	0.52
1:B:555:ASP:O	1:B:557:PRO:HD3	2.10	0.52
1:C:506:ALA:O	1:C:507:ALA:CB	2.58	0.52
1:C:647:VAL:HG23	1:C:647:VAL:O	2.10	0.52
1:D:265:VAL:HG13	1:D:265:VAL:O	2.08	0.52
1:D:291:ILE:N	1:D:291:ILE:HD12	2.24	0.52
1:A:308:THR:HG22	1:A:309:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1314:GLN:H	1:B:1314:GLN:CD	2.18	0.52
1:A:1110:ILE:O	1:A:1110:ILE:HG13	2.09	0.51
1:B:371:ILE:HA	1:B:374:ILE:HG22	1.92	0.51
1:B:507:ALA:HB1	1:B:508:PRO:HD2	1.92	0.51
1:B:659:TYR:HE2	1:B:819:VAL:HG21	1.74	0.51
1:B:967:THR:C	7:B:2131:HOH:O	2.52	0.51
1:C:33:TYR:CD1	1:C:37:VAL:HG11	2.44	0.51
1:C:216:LEU:HD12	1:C:216:LEU:N	2.26	0.51
1:C:1131:SER:HB2	1:D:1137:TYR:CD1	2.44	0.51
1:D:900:ARG:HH11	1:D:902:ARG:NH2	2.07	0.51
1:D:917:ARG:CZ	1:D:1203:ALA:HB2	2.40	0.51
1:D:1009:LYS:HD3	1:D:1158:PHE:CD2	2.45	0.51
1:A:514:TYR:CZ	1:A:518:LEU:HD11	2.45	0.51
1:A:524:PHE:O	1:A:527:TYR:HB3	2.11	0.51
1:B:92:VAL:HA	1:B:126:MET:CE	2.37	0.51
1:B:1009:LYS:HD3	1:B:1158:PHE:CD2	2.45	0.51
1:C:472:SER:OG	1:C:474:ASP:HB2	2.09	0.51
1:D:984:ASN:O	1:D:987:LYS:HB2	2.09	0.51
1:A:33:TYR:CD1	1:A:37:VAL:HG11	2.44	0.51
1:A:147:LEU:O	1:A:149:GLY:N	2.42	0.51
1:A:1009:LYS:HD3	1:A:1158:PHE:CD2	2.45	0.51
1:B:578:ASP:OD2	1:B:1057:ARG:NH1	2.43	0.51
1:B:992:PHE:CZ	1:B:996:ARG:HG3	2.45	0.51
1:C:387:ILE:HG22	1:C:388:GLN:N	2.25	0.51
1:D:676:ALA:HB3	1:D:682:ALA:HB2	1.92	0.51
1:A:467:GLY:HA3	1:A:471:ILE:CG2	2.40	0.51
1:A:945:LYS:O	1:A:949:LEU:HG	2.10	0.51
1:A:1000:LYS:HE2	1:A:1286:ALA:HA	1.92	0.51
1:B:483:ARG:NH2	1:B:489:MET:HA	2.26	0.51
1:B:797:LYS:HG3	1:B:1069:ASP:O	2.11	0.51
1:B:1106:LEU:O	1:B:1110:ILE:HG23	2.11	0.51
1:C:308:THR:HG22	1:C:309:GLY:N	2.26	0.51
1:D:776:PHE:CZ	1:D:780:MET:HE3	2.44	0.51
1:D:1111:LYS:O	1:D:1114:PRO:HD3	2.09	0.51
1:A:313:THR:HG23	7:A:2059:HOH:O	2.09	0.51
1:B:33:TYR:CD1	1:B:37:VAL:HG11	2.45	0.51
1:C:61:ARG:NH1	7:C:2010:HOH:O	2.40	0.51
1:C:514:TYR:CZ	1:C:518:LEU:HD11	2.46	0.51
1:C:524:PHE:O	1:C:527:TYR:HB3	2.11	0.51
1:C:1067:HIS:HE1	1:D:764:GLU:OE2	1.92	0.51
1:D:1069:ASP:N	7:D:2134:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ILE:N	1:A:291:ILE:HD12	2.26	0.51
1:A:1045:GLN:OE1	1:A:1045:GLN:N	2.33	0.51
1:B:291:ILE:HD12	1:B:291:ILE:N	2.26	0.51
1:B:552:ILE:HG22	1:B:998:TRP:HB2	1.91	0.51
1:B:916:PHE:C	5:B:3004:MOS:S	2.94	0.51
1:C:264:LEU:HD13	1:C:286:ILE:HB	1.93	0.51
1:C:380:ASN:ND2	7:C:2061:HOH:O	2.43	0.51
1:D:78:LEU:O	1:D:80:PRO:HD3	2.11	0.51
1:A:644:ALA:O	1:A:647:VAL:HG22	2.11	0.51
1:A:798:ARG:HG2	1:A:798:ARG:HH11	1.76	0.51
1:B:644:ALA:O	1:B:647:VAL:HG22	2.11	0.51
1:B:868:LEU:HD11	1:B:890:LEU:HD23	1.92	0.51
1:B:1000:LYS:HE2	1:B:1286:ALA:HA	1.93	0.51
1:D:66:SER:O	1:D:67:LYS:HB2	2.11	0.51
1:D:1025:LEU:HD13	1:D:1135:THR:HG22	1.93	0.51
1:D:1093:ARG:NH1	1:D:1093:ARG:HG3	2.23	0.51
1:A:112:GLY:HA3	7:A:2025:HOH:O	2.08	0.51
1:B:473:ALA:O	1:B:474:ASP:C	2.53	0.51
1:B:514:TYR:CZ	1:B:518:LEU:HD11	2.46	0.51
1:D:659:TYR:HE2	1:D:819:VAL:HG21	1.75	0.51
1:A:264:LEU:HD13	1:A:286:ILE:HB	1.93	0.51
1:B:524:PHE:O	1:B:527:TYR:HB3	2.11	0.51
1:C:568:GLN:N	7:C:2073:HOH:O	2.44	0.51
1:C:797:LYS:HG3	1:C:1069:ASP:O	2.10	0.51
1:A:790:ASN:OD1	1:A:791:ARG:HD3	2.11	0.51
1:C:506:ALA:CB	1:C:512:GLU:CD	2.81	0.51
1:C:591:LYS:HD3	1:D:761:GLU:HG3	1.91	0.51
1:D:201:LEU:CD1	1:D:565:GLN:HG3	2.40	0.51
1:D:772:GLN:HE22	1:D:804:GLY:HA2	1.76	0.51
1:A:987:LYS:HD2	7:A:2150:HOH:O	2.12	0.50
1:A:1296:TRP:N	7:A:2176:HOH:O	2.44	0.50
1:B:1196:ASP:HB3	1:B:1264:LEU:HD12	1.92	0.50
1:C:1314:GLN:CD	1:C:1314:GLN:H	2.18	0.50
1:D:1237:VAL:O	7:D:2150:HOH:O	2.18	0.50
1:A:659:TYR:HE2	1:A:819:VAL:HG21	1.75	0.50
1:A:1103:MET:HA	1:A:1103:MET:CE	2.40	0.50
1:C:1093:ARG:CG	1:C:1093:ARG:NH1	2.56	0.50
1:D:1000:LYS:HE2	1:D:1286:ALA:HA	1.92	0.50
1:A:507:ALA:HB1	1:A:508:PRO:HD2	1.93	0.50
1:A:632:ALA:O	1:A:635:SER:N	2.42	0.50
1:A:633:LEU:HD12	1:A:633:LEU:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ASN:HB3	1:A:1074:VAL:CG2	2.42	0.50
1:B:790:ASN:OD1	1:B:791:ARG:HD3	2.11	0.50
1:B:1058:GLU:OE1	1:B:1259:TYR:OH	2.29	0.50
1:A:776:PHE:CZ	1:A:780:MET:HE3	2.46	0.50
1:B:798:ARG:HH11	1:B:798:ARG:HG2	1.76	0.50
1:C:1137:TYR:CG	1:D:1131:SER:HB2	2.47	0.50
1:D:154:CYS:O	1:D:1202:GLY:HA3	2.11	0.50
1:D:1058:GLU:OE1	1:D:1259:TYR:OH	2.28	0.50
1:A:916:PHE:C	5:A:3004:MOS:S	2.95	0.50
1:A:987:LYS:NZ	7:A:2149:HOH:O	2.26	0.50
1:B:770:SER:N	7:B:2115:HOH:O	2.41	0.50
1:B:793:ASN:HB3	1:B:1074:VAL:CG2	2.41	0.50
1:C:614:VAL:HG12	1:C:673:ALA:CB	2.42	0.50
1:C:772:GLN:HE22	1:C:804:GLY:HA2	1.77	0.50
1:C:790:ASN:OD1	1:C:791:ARG:HD3	2.11	0.50
1:D:47:CYS:SG	1:D:1229:PRO:HG2	2.51	0.50
1:D:632:ALA:O	1:D:635:SER:N	2.43	0.50
1:D:760:GLY:O	7:D:2110:HOH:O	2.18	0.50
1:A:1077:PRO:CG	1:B:1027:GLN:HG3	2.39	0.50
1:B:863:ALA:HA	1:B:898:ASN:O	2.10	0.50
1:B:1025:LEU:HD13	1:B:1135:THR:HG22	1.94	0.50
1:C:676:ALA:HB3	1:C:682:ALA:HB2	1.94	0.50
1:C:868:LEU:HD11	1:C:890:LEU:HD23	1.93	0.50
1:D:467:GLY:HA3	1:D:471:ILE:CG2	2.42	0.50
1:A:358:HIS:NE2	1:A:366:SER:OG	2.31	0.50
1:A:647:VAL:HG23	1:A:647:VAL:O	2.12	0.50
1:A:910:LEU:HA	7:A:2117:HOH:O	2.11	0.50
1:B:148:GLY:CA	7:B:2029:HOH:O	2.59	0.50
1:B:580:ILE:HG13	1:B:1057:ARG:HG3	1.92	0.50
1:C:113:HIS:C	1:C:115:THR:H	2.20	0.50
1:A:529:ASP:HA	1:A:553:LEU:HD13	1.94	0.50
1:B:374:ILE:HG13	1:B:446:LYS:HB3	1.94	0.50
1:B:636:LEU:N	7:B:2096:HOH:O	2.45	0.50
1:C:319:LEU:HB3	1:C:338:LEU:CD2	2.42	0.50
1:C:924:GLY:C	7:C:2112:HOH:O	2.53	0.50
1:D:969:LEU:HB2	1:D:1160:PHE:CD1	2.47	0.50
1:A:559:THR:CB	1:A:1242:GLU:HB3	2.41	0.50
1:A:712:PHE:CG	1:A:904:ARG:HD3	2.47	0.50
1:B:307:GLY:HA2	1:B:413:SER:HB3	1.93	0.50
1:C:704:GLN:HE21	1:C:704:GLN:N	2.05	0.50
1:C:863:ALA:HA	1:C:898:ASN:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1023:ALA:HB3	1:C:1076:VAL:HG13	1.93	0.50
1:D:319:LEU:HB3	1:D:338:LEU:CD2	2.42	0.50
1:D:772:GLN:HE21	1:D:807:ALA:HB2	1.77	0.50
1:D:797:LYS:HG3	1:D:1069:ASP:O	2.12	0.50
1:A:33:TYR:HA	1:A:37:VAL:HG12	1.93	0.49
1:A:308:THR:HG21	6:A:3005:FAD:H62A	1.68	0.49
1:A:756:VAL:O	1:A:827:PRO:HA	2.12	0.49
1:A:1106:LEU:O	1:A:1110:ILE:HG23	2.11	0.49
1:B:264:LEU:HD13	1:B:286:ILE:HB	1.94	0.49
1:B:269:THR:HB	6:B:3005:FAD:HM83	1.94	0.49
1:B:362:ARG:NH1	1:B:403:ALA:N	2.60	0.49
1:B:1097:ASN:ND2	1:B:1137:TYR:H	2.07	0.49
1:C:264:LEU:O	6:C:3005:FAD:H2B	2.12	0.49
1:C:1077:PRO:HD3	1:D:1027:GLN:OE1	2.12	0.49
1:D:47:CYS:SG	1:D:48:GLY:N	2.82	0.49
1:D:839:LEU:HG	1:D:1227:ARG:HD3	1.94	0.49
1:A:955:ILE:HA	7:A:2144:HOH:O	2.12	0.49
1:A:1058:GLU:OE1	1:A:1259:TYR:OH	2.30	0.49
1:C:66:SER:O	1:C:67:LYS:HB2	2.12	0.49
1:C:291:ILE:N	1:C:291:ILE:HD12	2.27	0.49
1:C:1018:PHE:O	1:C:1021:GLN:HG2	2.12	0.49
1:D:790:ASN:OD1	1:D:791:ARG:HD3	2.11	0.49
1:A:578:ASP:OD2	1:A:1057:ARG:NH1	2.45	0.49
1:A:772:GLN:HE21	1:A:807:ALA:HB2	1.77	0.49
1:B:435:GLN:HG3	7:B:2029:HOH:O	2.11	0.49
1:B:632:ALA:O	1:B:635:SER:N	2.44	0.49
1:B:1208:LEU:HD12	1:B:1275:VAL:HG21	1.94	0.49
1:C:761:GLU:HG3	1:D:591:LYS:HD3	1.93	0.49
1:D:33:TYR:CD1	1:D:37:VAL:HG11	2.47	0.49
1:D:1018:PHE:O	1:D:1021:GLN:HG2	2.13	0.49
1:D:1023:ALA:HB3	1:D:1076:VAL:HG13	1.93	0.49
1:D:1048:ASN:O	1:D:1052:ILE:HG12	2.12	0.49
1:A:307:GLY:HA2	1:A:413:SER:HB3	1.93	0.49
1:A:1101:ILE:O	1:A:1105:ARG:HG3	2.12	0.49
1:C:367:ASP:CB	6:C:3005:FAD:O2	2.60	0.49
1:C:956:ASP:OD1	1:C:957:ARG:N	2.34	0.49
1:D:362:ARG:HA	7:D:2065:HOH:O	2.12	0.49
1:D:863:ALA:HA	1:D:898:ASN:O	2.11	0.49
1:A:143:ILE:O	1:A:146:THR:HG22	2.13	0.49
1:A:863:ALA:HA	1:A:898:ASN:O	2.12	0.49
1:A:984:ASN:O	1:A:987:LYS:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:529:ASP:HA	1:D:553:LEU:HD13	1.94	0.49
1:C:42:GLY:O	1:C:44:LYS:HE3	2.12	0.49
1:C:115:THR:CG2	1:C:592:HIS:ND1	2.76	0.49
1:C:147:LEU:O	1:C:149:GLY:N	2.45	0.49
1:C:580:ILE:HG13	1:C:1057:ARG:HG3	1.95	0.49
1:C:916:PHE:C	5:C:3004:MOS:S	2.96	0.49
1:C:1103:MET:HA	1:C:1103:MET:CE	2.40	0.49
1:C:1143:ALA:HB2	7:C:2132:HOH:O	2.11	0.49
1:D:580:ILE:HG13	1:D:1057:ARG:HG3	1.94	0.49
1:D:1208:LEU:HD12	1:D:1275:VAL:HG21	1.93	0.49
1:A:1219:SER:OG	1:A:1223:VAL:CG1	2.59	0.49
1:B:153:ARG:HH22	1:B:744:GLN:HE21	1.60	0.49
1:B:667:VAL:HB	7:B:2103:HOH:O	2.11	0.49
1:B:1101:ILE:O	1:B:1105:ARG:HG3	2.13	0.49
1:D:115:THR:CG2	1:D:592:HIS:ND1	2.76	0.49
1:D:576:LEU:HA	1:D:582:ARG:NH2	2.28	0.49
1:D:712:PHE:CG	1:D:904:ARG:HD3	2.48	0.49
1:D:910:LEU:CD1	1:D:1334:VAL:HG11	2.43	0.49
1:A:797:LYS:HG3	1:A:1069:ASP:O	2.13	0.49
1:A:868:LEU:HD11	1:A:890:LEU:HD23	1.94	0.49
1:B:467:GLY:HA3	1:B:471:ILE:CG2	2.43	0.49
1:C:844:ARG:NH1	1:C:916:PHE:HB3	2.28	0.49
1:C:945:LYS:O	1:C:949:LEU:HG	2.13	0.49
1:D:868:LEU:HD11	1:D:890:LEU:HD23	1.95	0.49
1:D:916:PHE:C	5:D:3004:MOS:S	2.96	0.49
1:D:955:ILE:HG22	7:D:2119:HOH:O	2.13	0.49
1:A:1208:LEU:HD12	1:A:1275:VAL:HG21	1.95	0.49
1:B:63:ASP:O	1:B:67:LYS:N	2.42	0.49
1:B:66:SER:O	1:B:67:LYS:HB2	2.12	0.49
1:C:798:ARG:HG2	1:C:798:ARG:HH11	1.77	0.49
1:C:804:GLY:HA2	5:C:3004:MOS:O1	2.12	0.49
1:C:1048:ASN:O	1:C:1052:ILE:HG12	2.13	0.49
1:C:1058:GLU:OE1	1:C:1259:TYR:OH	2.30	0.49
1:D:578:ASP:OD2	1:D:1057:ARG:NH1	2.45	0.49
1:D:644:ALA:O	1:D:647:VAL:HG22	2.12	0.49
1:D:704:GLN:O	1:D:708:GLN:HG2	2.13	0.49
1:A:32:PHE:CE1	1:A:36:LYS:HG3	2.48	0.49
1:A:137:GLU:OE1	1:D:68:ARG:NH2	2.46	0.49
1:A:753:SER:HB3	1:A:831:ILE:CD1	2.43	0.49
1:A:770:SER:O	1:A:806:LYS:HD3	2.13	0.49
1:A:1111:LYS:HA	1:A:1111:LYS:HD3	1.67	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1227:ARG:NH2	7:A:2173:HOH:O	2.45	0.49
1:B:47:CYS:SG	1:B:1229:PRO:HG2	2.52	0.49
1:B:265:VAL:HG13	1:B:265:VAL:O	2.13	0.49
1:B:559:THR:CB	1:B:1242:GLU:HB3	2.43	0.49
1:B:609:GLU:HA	1:B:827:PRO:HG2	1.95	0.49
1:B:676:ALA:HB3	1:B:682:ALA:HB2	1.94	0.49
1:B:712:PHE:CG	1:B:904:ARG:HD3	2.47	0.49
1:B:1023:ALA:HB3	1:B:1076:VAL:CG1	2.43	0.49
1:B:1048:ASN:O	1:B:1052:ILE:HG12	2.12	0.49
1:C:761:GLU:HG3	1:D:591:LYS:HD2	1.95	0.49
1:C:772:GLN:HE21	1:C:807:ALA:HB2	1.78	0.49
1:D:486:ASP:OD1	1:D:486:ASP:N	2.46	0.49
1:D:1152:GLY:HA2	7:D:2142:HOH:O	2.13	0.49
1:C:381:VAL:HG13	7:C:2060:HOH:O	2.13	0.48
1:B:771:SER:HB3	7:B:2115:HOH:O	2.13	0.48
1:C:78:LEU:O	1:C:80:PRO:HD3	2.13	0.48
1:C:1106:LEU:O	1:C:1110:ILE:HG23	2.13	0.48
1:D:371:ILE:HA	1:D:374:ILE:HG22	1.95	0.48
1:D:580:ILE:HG12	1:D:1057:ARG:HG3	1.94	0.48
1:A:113:HIS:C	1:A:115:THR:H	2.20	0.48
1:A:1219:SER:HB3	1:A:1225:TYR:CZ	2.49	0.48
1:B:770:SER:O	1:B:806:LYS:HD3	2.13	0.48
1:B:772:GLN:NE2	1:B:807:ALA:HB2	2.29	0.48
1:C:1101:ILE:O	1:C:1105:ARG:HG3	2.12	0.48
1:C:1142:GLN:O	7:C:2132:HOH:O	2.20	0.48
1:D:33:TYR:HA	1:D:37:VAL:HG12	1.95	0.48
1:D:44:LYS:HE2	1:D:44:LYS:HB3	1.74	0.48
1:B:33:TYR:O	1:B:37:VAL:HG12	2.13	0.48
1:B:772:GLN:HE22	1:B:804:GLY:HA2	1.77	0.48
1:B:772:GLN:HE21	1:B:807:ALA:HB2	1.78	0.48
1:B:839:LEU:HG	1:B:1227:ARG:HD3	1.94	0.48
1:C:217:ILE:O	1:C:218:PHE:C	2.56	0.48
1:C:888:LEU:HD13	1:C:1154:ILE:CD1	2.43	0.48
1:C:1208:LEU:HD12	1:C:1275:VAL:HG21	1.94	0.48
1:D:483:ARG:NH2	1:D:489:MET:HA	2.28	0.48
1:D:770:SER:O	1:D:806:LYS:HD3	2.13	0.48
1:A:104:PRO:O	1:A:108:ARG:HG3	2.13	0.48
1:A:772:GLN:NE2	1:A:807:ALA:HB2	2.28	0.48
1:A:839:LEU:HG	1:A:1227:ARG:HD3	1.95	0.48
1:B:576:LEU:HA	1:B:582:ARG:NH2	2.28	0.48
1:B:633:LEU:HD12	1:B:633:LEU:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1043:LEU:HG	1:B:1045:GLN:HE22	1.78	0.48
1:D:16:GLY:N	7:D:2003:HOH:O	2.12	0.48
1:D:932:MET:HE3	1:D:946:VAL:HG12	1.94	0.48
1:A:33:TYR:O	1:A:37:VAL:HG12	2.13	0.48
1:A:353:ALA:HB1	6:A:3005:FAD:H4'	1.95	0.48
1:A:772:GLN:HE22	1:A:804:GLY:HA2	1.78	0.48
1:A:805:GLY:O	7:A:2128:HOH:O	2.20	0.48
1:B:1093:ARG:HG3	1:B:1093:ARG:NH1	2.23	0.48
1:C:344:LEU:HD13	6:C:3005:FAD:C10	2.43	0.48
1:C:741:LEU:HA	1:C:1300:SER:CB	2.44	0.48
1:C:767:ILE:HD12	1:C:792:ILE:HD12	1.96	0.48
1:C:1219:SER:OG	1:C:1223:VAL:CG1	2.62	0.48
1:D:358:HIS:HB2	6:D:3005:FAD:O4'	2.13	0.48
1:A:970:LEU:O	1:A:974:GLU:HG2	2.14	0.48
1:B:529:ASP:HA	1:B:553:LEU:HD13	1.95	0.48
1:B:615:VAL:HG13	1:B:672:CYS:SG	2.53	0.48
1:B:844:ARG:NH2	1:B:916:PHE:CD1	2.81	0.48
1:C:472:SER:C	1:C:474:ASP:H	2.21	0.48
1:C:636:LEU:N	7:C:2082:HOH:O	2.47	0.48
1:C:1196:ASP:HB3	1:C:1264:LEU:HD12	1.96	0.48
1:D:51:ASP:HB3	1:D:1229:PRO:HB2	1.96	0.48
1:A:78:LEU:O	1:A:80:PRO:HD3	2.14	0.48
1:A:741:LEU:HA	1:A:1300:SER:CB	2.42	0.48
1:B:319:LEU:HB3	1:B:338:LEU:CD2	2.43	0.48
1:B:916:PHE:O	1:B:917:ARG:C	2.56	0.48
1:C:216:LEU:HD12	1:C:216:LEU:H	1.79	0.48
1:C:932:MET:HE3	1:C:946:VAL:HG12	1.95	0.48
1:C:984:ASN:O	1:C:987:LYS:HB2	2.13	0.48
1:D:58:MET:CG	7:D:2013:HOH:O	2.49	0.48
1:D:798:ARG:HG2	1:D:798:ARG:NH1	2.28	0.48
1:D:1238:THR:OG1	7:D:2072:HOH:O	2.02	0.48
1:A:265:VAL:O	1:A:265:VAL:HG13	2.13	0.48
1:C:659:TYR:HE2	1:C:819:VAL:HG21	1.77	0.48
1:D:307:GLY:HA2	1:D:413:SER:HB3	1.95	0.48
1:D:594:THR:OG1	1:D:596:GLU:HG3	2.14	0.48
1:D:1106:LEU:O	1:D:1110:ILE:HG23	2.14	0.48
1:A:39:ARG:HG2	7:A:2009:HOH:O	2.14	0.48
1:B:932:MET:HE3	1:B:946:VAL:HG12	1.96	0.48
1:C:1025:LEU:HD13	1:C:1135:THR:HG22	1.96	0.48
1:D:615:VAL:HG13	1:D:672:CYS:SG	2.54	0.48
1:A:75:THR:O	1:A:79:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:TYR:CD1	1:B:562:TYR:C	2.92	0.47
1:C:1093:ARG:HG3	1:C:1093:ARG:NH1	2.24	0.47
1:A:580:ILE:HG13	1:A:1057:ARG:HG3	1.96	0.47
1:A:844:ARG:NH2	1:A:916:PHE:CD1	2.82	0.47
1:B:36:LYS:HE3	7:B:2010:HOH:O	2.13	0.47
1:B:103:HIS:CE1	1:B:105:VAL:HG23	2.49	0.47
1:C:644:ALA:O	1:C:647:VAL:HG22	2.14	0.47
1:D:677:ASP:OD2	7:D:2101:HOH:O	2.19	0.47
1:D:844:ARG:NH2	1:D:916:PHE:CD1	2.82	0.47
1:A:932:MET:HE3	1:A:946:VAL:HG12	1.96	0.47
1:B:303:GLY:HA3	1:B:415:PHE:CE1	2.48	0.47
1:B:568:GLN:NE2	7:B:2078:HOH:O	2.47	0.47
1:C:33:TYR:O	1:C:37:VAL:HG12	2.14	0.47
1:C:75:THR:O	1:C:79:VAL:HG23	2.14	0.47
1:D:753:SER:HB3	1:D:831:ILE:CD1	2.43	0.47
1:D:772:GLN:NE2	1:D:807:ALA:HB2	2.29	0.47
1:A:63:ASP:O	1:A:67:LYS:N	2.37	0.47
1:A:390:ILE:HB	7:A:2069:HOH:O	2.14	0.47
1:A:1023:ALA:HB3	1:A:1076:VAL:CG1	2.45	0.47
1:B:78:LEU:O	1:B:80:PRO:HD3	2.14	0.47
1:C:490:LEU:HD12	1:C:527:TYR:CD2	2.49	0.47
1:C:576:LEU:HA	1:C:582:ARG:NH2	2.28	0.47
1:C:839:LEU:HG	1:C:1227:ARG:HD3	1.96	0.47
1:C:1138:PHE:CE2	1:C:1140:GLY:HA2	2.49	0.47
1:A:727:ALA:HA	1:A:730:CYS:SG	2.55	0.47
1:A:967:THR:HA	7:A:2148:HOH:O	2.13	0.47
1:B:113:HIS:C	1:B:115:THR:H	2.22	0.47
1:B:746:HIS:HA	1:B:916:PHE:CE2	2.50	0.47
1:B:779:GLU:HB3	1:B:789:LYS:HE3	1.96	0.47
1:B:1018:PHE:O	1:B:1021:GLN:HG2	2.14	0.47
1:C:719:LEU:CD1	1:C:888:LEU:HD23	2.44	0.47
1:C:727:ALA:HA	1:C:730:CYS:SG	2.54	0.47
1:D:91:THR:HG23	7:D:2004:HOH:O	2.13	0.47
1:A:130:THR:HA	7:A:2015:HOH:O	2.14	0.47
1:A:153:ARG:HH22	1:A:744:GLN:HE21	1.62	0.47
1:A:549:LEU:HD23	7:A:2086:HOH:O	2.13	0.47
1:B:308:THR:HG22	1:B:309:GLY:N	2.27	0.47
1:B:490:LEU:HD12	1:B:527:TYR:CD2	2.50	0.47
1:B:713:ILE:CG1	1:B:907:LYS:HB3	2.31	0.47
1:C:216:LEU:H	1:C:216:LEU:CD1	2.26	0.47
1:C:910:LEU:CD1	1:C:1334:VAL:HG11	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NH2	1:D:137:GLU:OE1	2.47	0.47
1:A:103:HIS:CE1	1:A:105:VAL:HG23	2.49	0.47
1:A:199:THR:OG1	1:A:200:LYS:N	2.47	0.47
1:A:319:LEU:HB3	1:A:338:LEU:CD2	2.43	0.47
1:A:319:LEU:O	1:A:323:VAL:HG22	2.15	0.47
1:A:746:HIS:HA	1:A:916:PHE:CZ	2.50	0.47
1:B:47:CYS:CB	1:B:1229:PRO:HG2	2.43	0.47
1:B:51:ASP:HB3	1:B:1229:PRO:HB2	1.97	0.47
1:B:433:ARG:NH1	1:B:1234:ILE:O	2.48	0.47
1:B:552:ILE:HG22	1:B:998:TRP:CB	2.45	0.47
1:B:712:PHE:HB3	1:B:904:ARG:HH11	1.80	0.47
1:B:727:ALA:HA	1:B:730:CYS:SG	2.54	0.47
1:B:970:LEU:O	1:B:974:GLU:HG2	2.15	0.47
1:B:1219:SER:OG	1:B:1223:VAL:CG1	2.61	0.47
1:C:374:ILE:HG13	1:C:446:LYS:HB3	1.96	0.47
1:C:632:ALA:O	1:C:633:LEU:C	2.58	0.47
1:C:633:LEU:HD12	1:C:633:LEU:H	1.78	0.47
1:C:779:GLU:HB3	1:C:789:LYS:HE3	1.96	0.47
1:A:242:THR:O	1:A:242:THR:HG22	2.15	0.47
1:B:1011:SER:HB3	1:B:1158:PHE:CD2	2.50	0.47
1:C:32:PHE:CE1	1:C:36:LYS:HG3	2.50	0.47
1:D:299:ASN:O	1:D:299:ASN:CG	2.58	0.47
1:D:713:ILE:CG1	1:D:907:LYS:HB3	2.30	0.47
1:D:779:GLU:HB3	1:D:789:LYS:HE3	1.97	0.47
1:A:490:LEU:HD12	1:A:527:TYR:CD2	2.49	0.47
1:A:490:LEU:C	1:A:490:LEU:CD2	2.88	0.47
1:A:691:ILE:HD11	1:A:693:TYR:CE1	2.49	0.47
1:B:435:GLN:HG2	1:B:436:ASN:N	2.30	0.47
1:B:753:SER:HB3	1:B:831:ILE:CD1	2.45	0.47
1:B:888:LEU:HD13	1:B:1154:ILE:CD1	2.44	0.47
1:D:33:TYR:O	1:D:37:VAL:CG1	2.63	0.47
1:D:287:SER:CB	7:D:2051:HOH:O	2.59	0.47
1:D:319:LEU:O	1:D:323:VAL:HG13	2.15	0.47
1:D:1239:ASP:OD1	7:D:2072:HOH:O	2.20	0.47
1:A:779:GLU:HB3	1:A:789:LYS:HE3	1.97	0.47
1:B:861:ILE:HD11	1:B:935:VAL:HG21	1.97	0.47
1:C:490:LEU:C	1:C:490:LEU:CD2	2.89	0.47
1:C:632:ALA:O	1:C:635:SER:N	2.44	0.47
1:C:924:GLY:CA	7:C:2112:HOH:O	2.63	0.47
1:D:435:GLN:HG2	1:D:436:ASN:N	2.29	0.47
1:A:632:ALA:O	1:A:633:LEU:C	2.57	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:LEU:HD13	1:A:1154:ILE:CD1	2.45	0.46
1:C:143:ILE:O	1:C:146:THR:HG22	2.15	0.46
1:C:970:LEU:O	1:C:974:GLU:HG2	2.15	0.46
1:C:1172:LEU:O	1:C:1308:ARG:NE	2.48	0.46
1:D:408:GLU:H	1:D:408:GLU:HG3	1.54	0.46
1:D:967:THR:N	7:D:2124:HOH:O	2.48	0.46
1:A:733:GLN:OE1	1:A:857:ASN:ND2	2.47	0.46
1:A:767:ILE:HD12	1:A:792:ILE:HD12	1.97	0.46
1:A:871:ASN:HD21	1:A:908:THR:HG21	1.81	0.46
1:B:143:ILE:O	1:B:146:THR:HG22	2.15	0.46
1:B:217:ILE:O	1:B:218:PHE:C	2.57	0.46
1:B:370:PRO:HG3	1:B:470:VAL:HG11	1.98	0.46
1:B:387:ILE:H	1:B:387:ILE:CD1	2.28	0.46
1:B:741:LEU:HA	1:B:1300:SER:CB	2.43	0.46
1:C:615:VAL:HG13	1:C:672:CYS:SG	2.55	0.46
1:C:868:LEU:HD11	1:C:890:LEU:CD2	2.45	0.46
1:C:924:GLY:HA2	7:C:2112:HOH:O	2.14	0.46
1:D:39:ARG:HB3	7:D:2009:HOH:O	2.14	0.46
1:D:793:ASN:HB3	1:D:1074:VAL:CG2	2.45	0.46
1:A:1169:ILE:HG12	1:A:1282:ALA:HB1	1.98	0.46
1:B:580:ILE:HG12	1:B:1057:ARG:HG3	1.96	0.46
1:B:614:VAL:HG12	1:B:673:ALA:CB	2.45	0.46
1:C:232:THR:H	1:C:290:ARG:HH22	1.63	0.46
1:C:319:LEU:O	1:C:323:VAL:HG22	2.15	0.46
1:D:520:ILE:O	1:D:523:LEU:HB3	2.14	0.46
1:D:551:HIS:CD2	1:D:996:ARG:CZ	2.98	0.46
1:D:1219:SER:HB3	1:D:1225:TYR:CZ	2.50	0.46
1:A:591:LYS:HD2	1:B:761:GLU:HG3	1.97	0.46
1:A:1025:LEU:HD13	1:A:1135:THR:CG2	2.45	0.46
1:B:594:THR:OG1	1:B:596:GLU:HG3	2.15	0.46
1:B:802:ALA:HB3	1:B:1043:LEU:HD13	1.97	0.46
1:B:1146:ASP:OD2	1:B:1149:LYS:HB2	2.16	0.46
1:C:1067:HIS:CE1	1:D:764:GLU:OE2	2.69	0.46
1:D:11:ILE:C	7:D:2002:HOH:O	2.50	0.46
1:D:113:HIS:C	1:D:115:THR:H	2.23	0.46
1:A:319:LEU:HD12	1:A:319:LEU:HA	1.74	0.46
1:A:1093:ARG:HD2	7:A:2167:HOH:O	2.16	0.46
1:B:314:GLN:NE2	7:B:2052:HOH:O	2.47	0.46
1:C:890:LEU:HD12	1:C:891:GLU:N	2.30	0.46
1:D:217:ILE:O	1:D:218:PHE:C	2.59	0.46
1:D:871:ASN:HD21	1:D:908:THR:HG21	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:880:GLU:CD	1:A:880:GLU:N	2.74	0.46
1:A:1138:PHE:CE2	1:A:1140:GLY:HA2	2.51	0.46
1:B:1185:MET:N	7:B:2158:HOH:O	2.00	0.46
1:C:753:SER:HB3	1:C:831:ILE:CD1	2.44	0.46
1:D:58:MET:CA	7:D:2012:HOH:O	2.64	0.46
1:D:742:GLY:O	7:D:2106:HOH:O	2.20	0.46
1:D:1023:ALA:HB3	1:D:1076:VAL:CG1	2.46	0.46
1:D:1103:MET:HA	1:D:1103:MET:CE	2.42	0.46
1:A:232:THR:H	1:A:290:ARG:HH22	1.64	0.46
1:A:667:VAL:HG11	1:A:1223:VAL:HA	1.98	0.46
1:B:557:PRO:HD2	7:B:2075:HOH:O	2.16	0.46
1:C:156:GLY:O	1:C:157:TYR:HB2	2.16	0.46
1:C:361:SER:O	1:C:362:ARG:C	2.58	0.46
1:C:703:VAL:HG13	1:C:704:GLN:HE22	1.80	0.46
6:C:3005:FAD:H9	6:C:3005:FAD:O3'	2.15	0.46
1:D:46:GLY:O	1:D:834:ARG:NE	2.38	0.46
1:D:153:ARG:HH22	1:D:744:GLN:HE21	1.63	0.46
1:D:633:LEU:HD12	1:D:633:LEU:H	1.79	0.46
1:A:802:ALA:HB3	1:A:1043:LEU:HD13	1.96	0.46
1:B:490:LEU:C	1:B:490:LEU:CD2	2.89	0.46
1:C:772:GLN:NE2	1:C:807:ALA:HB2	2.31	0.46
1:C:992:PHE:CZ	1:C:996:ARG:HG3	2.50	0.46
1:C:1027:GLN:OE1	1:D:1077:PRO:HD3	2.14	0.46
1:A:844:ARG:NH1	1:A:916:PHE:HB3	2.31	0.46
1:B:804:GLY:HA2	5:B:3004:MOS:O1	2.16	0.46
1:C:986:LYS:CB	7:C:2114:HOH:O	2.64	0.46
1:D:259:HIS:ND1	7:D:2047:HOH:O	2.20	0.46
1:D:970:LEU:O	1:D:974:GLU:HG2	2.16	0.46
1:A:346:GLY:C	7:A:2064:HOH:O	2.59	0.46
1:A:369:ASN:HB2	1:A:370:PRO:HD3	1.98	0.46
1:A:861:ILE:HD11	1:A:935:VAL:HG21	1.97	0.46
1:A:1131:SER:HB2	1:B:1137:TYR:CD1	2.51	0.46
1:B:319:LEU:O	1:B:323:VAL:HG22	2.16	0.46
1:B:980:SER:HB2	1:B:985:ARG:HH21	1.81	0.46
1:C:606:LEU:HD23	1:D:606:LEU:HD23	1.97	0.46
1:D:143:ILE:O	1:D:146:THR:HG22	2.16	0.46
1:D:271:LEU:O	1:D:275:MET:HB2	2.15	0.46
1:D:528:LEU:HB2	1:D:553:LEU:HD21	1.98	0.46
1:D:703:VAL:HG23	1:D:906:CYS:SG	2.56	0.46
1:A:370:PRO:HG3	1:A:470:VAL:HG11	1.98	0.45
1:B:474:ASP:HA	1:B:477:CYS:HG	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:HIS:HA	1:B:916:PHE:CZ	2.50	0.45
1:B:868:LEU:HD11	1:B:890:LEU:CD2	2.46	0.45
1:C:844:ARG:NH2	1:C:916:PHE:CD1	2.83	0.45
1:C:1021:GLN:HA	1:C:1138:PHE:O	2.15	0.45
1:D:75:THR:O	1:D:79:VAL:HG23	2.15	0.45
1:D:727:ALA:HA	1:D:730:CYS:SG	2.56	0.45
1:D:888:LEU:HD13	1:D:1154:ILE:CD1	2.46	0.45
1:A:66:SER:O	1:A:67:LYS:CB	2.64	0.45
1:A:659:TYR:CE2	1:A:819:VAL:HG21	2.51	0.45
1:A:709:TYR:O	1:A:710:GLU:C	2.59	0.45
1:A:712:PHE:HB3	1:A:904:ARG:HH11	1.80	0.45
1:A:767:ILE:HD12	1:A:792:ILE:CD1	2.47	0.45
1:B:199:THR:OG1	1:B:200:LYS:N	2.46	0.45
1:B:397:LEU:HD22	1:B:470:VAL:HG21	1.99	0.45
1:B:703:VAL:HG23	1:B:906:CYS:SG	2.55	0.45
1:B:910:LEU:CD1	1:B:1334:VAL:HG11	2.46	0.45
1:B:1037:ALA:HB2	7:B:2142:HOH:O	2.16	0.45
1:B:1233:LYS:NZ	7:B:2016:HOH:O	2.49	0.45
1:C:871:ASN:HD21	1:C:908:THR:HG21	1.80	0.45
1:C:1294:PRO:O	1:C:1295:ILE:C	2.59	0.45
1:D:147:LEU:C	1:D:149:GLY:N	2.72	0.45
1:D:433:ARG:NH1	1:D:1234:ILE:O	2.49	0.45
1:D:627:LEU:HD13	1:D:627:LEU:C	2.41	0.45
1:A:58:MET:CG	7:A:2015:HOH:O	2.54	0.45
1:B:84:LEU:O	1:B:85:HIS:C	2.59	0.45
1:C:103:HIS:CG	1:C:104:PRO:HD2	2.51	0.45
1:C:986:LYS:HB3	7:C:2114:HOH:O	2.15	0.45
1:D:369:ASN:HB2	1:D:370:PRO:HD3	1.98	0.45
1:D:632:ALA:O	1:D:633:LEU:C	2.59	0.45
1:A:147:LEU:C	1:A:149:GLY:N	2.74	0.45
1:A:674:VAL:HG11	1:A:686:ALA:HB2	1.98	0.45
1:A:712:PHE:CB	1:A:904:ARG:NH1	2.80	0.45
1:B:712:PHE:CB	1:B:904:ARG:NH1	2.80	0.45
1:B:719:LEU:CD1	1:B:888:LEU:HD23	2.46	0.45
1:B:879:SER:HB3	1:B:905:VAL:HG11	1.99	0.45
1:C:667:VAL:HG11	1:C:1223:VAL:HA	1.99	0.45
1:C:792:ILE:O	1:C:792:ILE:HG12	2.17	0.45
1:C:839:LEU:HD23	1:C:839:LEU:HA	1.86	0.45
1:C:1097:ASN:ND2	1:C:1137:TYR:H	2.08	0.45
1:D:10:LEU:HD22	7:D:2020:HOH:O	2.16	0.45
1:D:317:ASN:ND2	7:D:2059:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:PHE:HB3	1:D:904:ARG:HH11	1.81	0.45
1:D:719:LEU:CD1	1:D:888:LEU:HD23	2.47	0.45
1:D:746:HIS:HA	1:D:916:PHE:CZ	2.51	0.45
1:D:1025:LEU:HD13	1:D:1135:THR:CG2	2.46	0.45
1:D:1138:PHE:CE2	1:D:1140:GLY:HA2	2.52	0.45
1:A:42:GLY:O	1:A:44:LYS:HE3	2.17	0.45
1:A:580:ILE:HG12	1:A:1057:ARG:HG3	1.99	0.45
1:A:719:LEU:CD1	1:A:888:LEU:HD23	2.46	0.45
1:A:1027:GLN:OE1	1:B:1077:PRO:HD3	2.17	0.45
1:B:50:GLY:HA2	3:B:3002:FES:S2	2.57	0.45
1:B:474:ASP:HA	1:B:477:CYS:SG	2.57	0.45
1:B:890:LEU:HD12	1:B:891:GLU:N	2.31	0.45
1:B:893:ALA:HB1	1:B:969:LEU:HD11	1.98	0.45
1:B:1169:ILE:HG12	1:B:1282:ALA:HB1	1.98	0.45
1:C:44:LYS:HE2	1:C:44:LYS:HB3	1.74	0.45
1:C:319:LEU:HB3	1:C:338:LEU:HD23	1.99	0.45
1:D:147:LEU:O	1:D:148:GLY:C	2.60	0.45
1:D:147:LEU:C	1:D:149:GLY:H	2.24	0.45
1:D:1011:SER:HB3	1:D:1158:PHE:CD2	2.52	0.45
1:D:1083:GLY:HA2	4:D:3003:MTE:S2'	2.57	0.45
1:A:980:SER:HB2	1:A:985:ARG:HH21	1.81	0.45
1:A:1097:ASN:ND2	1:A:1137:TYR:H	2.09	0.45
1:C:319:LEU:O	1:C:323:VAL:HG13	2.16	0.45
1:C:319:LEU:HD12	1:C:319:LEU:HA	1.76	0.45
1:C:627:LEU:HD13	1:C:627:LEU:C	2.42	0.45
1:C:1011:SER:HB3	1:C:1158:PHE:CD2	2.52	0.45
1:D:66:SER:O	1:D:67:LYS:CB	2.65	0.45
1:D:358:HIS:CB	6:D:3005:FAD:O4'	2.65	0.45
1:D:879:SER:HB3	1:D:905:VAL:HG11	1.98	0.45
1:A:798:ARG:HG2	1:A:798:ARG:NH1	2.31	0.45
1:A:804:GLY:HA2	5:A:3004:MOS:O1	2.16	0.45
1:B:816:VAL:O	1:B:819:VAL:HG22	2.17	0.45
1:B:1219:SER:HB3	1:B:1225:TYR:CZ	2.52	0.45
1:A:1048:ASN:O	1:A:1052:ILE:HG12	2.16	0.45
1:B:147:LEU:C	1:B:149:GLY:N	2.74	0.45
1:B:691:ILE:HD11	1:B:693:TYR:CE1	2.52	0.45
1:C:370:PRO:HG3	1:C:470:VAL:HG11	1.97	0.45
1:C:507:ALA:HB1	1:C:508:PRO:CD	2.46	0.45
1:C:580:ILE:HG12	1:C:1057:ARG:HG3	1.98	0.45
1:D:85:HIS:CA	7:D:2002:HOH:O	2.59	0.45
1:D:308:THR:HG22	1:D:309:GLY:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:674:VAL:HG11	1:D:686:ALA:HB2	1.98	0.45
1:D:890:LEU:HD12	1:D:891:GLU:N	2.32	0.45
1:A:712:PHE:HB3	1:A:904:ARG:NH1	2.31	0.45
1:A:1172:LEU:O	1:A:1308:ARG:NE	2.50	0.45
1:B:33:TYR:O	1:B:37:VAL:CG1	2.65	0.45
1:C:369:ASN:HB2	1:C:370:PRO:HD3	1.99	0.45
1:C:861:ILE:HD11	1:C:935:VAL:HG21	1.98	0.45
1:C:980:SER:HB2	1:C:985:ARG:HH21	1.81	0.45
1:D:992:PHE:CZ	1:D:996:ARG:HG3	2.52	0.45
1:A:116:GLN:HB3	1:A:1044:GLY:O	2.17	0.45
1:A:967:THR:CA	7:A:2148:HOH:O	2.64	0.45
1:A:1103:MET:HE1	1:A:1118:TRP:HZ3	1.82	0.45
1:B:156:GLY:O	1:B:157:TYR:HB2	2.17	0.45
1:B:1103:MET:HA	1:B:1103:MET:CE	2.42	0.45
1:D:58:MET:N	7:D:2012:HOH:O	2.49	0.45
1:D:199:THR:OG1	1:D:200:LYS:N	2.46	0.45
1:D:275:MET:HG2	1:D:282:TYR:CE2	2.51	0.45
1:D:370:PRO:HG3	1:D:470:VAL:HG11	1.98	0.45
1:D:659:TYR:CE2	1:D:819:VAL:HG21	2.52	0.45
1:D:1006:ILE:HD11	1:D:1271:LEU:HA	1.99	0.45
1:A:844:ARG:HG2	1:A:923:GLN:NE2	2.32	0.44
1:B:147:LEU:C	1:B:149:GLY:H	2.25	0.44
1:B:659:TYR:CE2	1:B:819:VAL:HG21	2.51	0.44
1:B:1021:GLN:HA	1:B:1138:PHE:O	2.18	0.44
1:C:199:THR:OG1	1:C:200:LYS:N	2.49	0.44
1:C:691:ILE:HD11	1:C:693:TYR:CE1	2.51	0.44
1:C:746:HIS:HA	1:C:916:PHE:CZ	2.52	0.44
1:C:798:ARG:HG2	1:C:798:ARG:NH1	2.32	0.44
1:C:879:SER:HB3	1:C:905:VAL:HG11	1.97	0.44
1:C:1243:GLU:HG2	1:C:1245:HIS:HE2	1.82	0.44
1:D:86:GLY:N	7:D:2002:HOH:O	2.45	0.44
1:D:667:VAL:HG11	1:D:1223:VAL:HA	1.99	0.44
1:D:1172:LEU:O	1:D:1308:ARG:NE	2.50	0.44
1:A:435:GLN:HG2	1:A:436:ASN:N	2.32	0.44
1:A:1011:SER:HB3	1:A:1158:PHE:CD2	2.52	0.44
1:B:627:LEU:C	1:B:627:LEU:HD13	2.43	0.44
1:B:1103:MET:HE1	1:B:1118:TRP:HZ3	1.81	0.44
1:C:395:HIS:C	1:C:397:LEU:N	2.72	0.44
1:C:429:ARG:NH2	1:C:437:ALA:O	2.50	0.44
1:C:802:ALA:HB3	1:C:1043:LEU:HD13	1.98	0.44
1:D:63:ASP:O	1:D:67:LYS:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:727:ALA:HB2	1:D:898:ASN:HD22	1.80	0.44
1:A:861:ILE:CG2	1:A:896:ILE:HD12	2.47	0.44
1:A:868:LEU:HD11	1:A:890:LEU:CD2	2.46	0.44
1:B:397:LEU:HD22	1:B:470:VAL:CG2	2.48	0.44
1:B:667:VAL:HG11	1:B:1223:VAL:HA	2.00	0.44
1:C:147:LEU:C	1:C:149:GLY:N	2.75	0.44
1:D:319:LEU:O	1:D:323:VAL:HG22	2.17	0.44
1:D:545:ILE:HG23	1:D:545:ILE:O	2.17	0.44
1:D:802:ALA:HB3	1:D:1043:LEU:HD13	1.99	0.44
1:D:804:GLY:HA2	5:D:3004:MOS:O1	2.17	0.44
1:A:349:ILE:HD13	1:A:349:ILE:HA	1.83	0.44
1:A:816:VAL:O	1:A:819:VAL:HG22	2.17	0.44
1:B:361:SER:O	1:B:362:ARG:C	2.60	0.44
1:B:369:ASN:HB2	1:B:370:PRO:HD3	1.99	0.44
1:B:709:TYR:O	1:B:710:GLU:C	2.60	0.44
1:B:900:ARG:NH1	1:B:902:ARG:NH2	2.60	0.44
1:B:1185:MET:SD	1:B:1267:ALA:HB1	2.58	0.44
1:C:1185:MET:SD	1:C:1267:ALA:HB1	2.57	0.44
1:C:1219:SER:HB3	1:C:1225:TYR:CZ	2.52	0.44
1:D:232:THR:H	1:D:290:ARG:HH22	1.65	0.44
1:D:723:ASN:HB2	7:D:2105:HOH:O	2.17	0.44
1:A:909:ASN:O	7:A:2117:HOH:O	2.21	0.44
1:A:910:LEU:CD1	1:A:1334:VAL:HG11	2.47	0.44
1:A:950:ASN:N	7:A:2143:HOH:O	2.50	0.44
1:B:712:PHE:HB3	1:B:904:ARG:NH1	2.33	0.44
1:B:1006:ILE:HD11	1:B:1271:LEU:HA	1.99	0.44
1:B:1172:LEU:O	1:B:1308:ARG:NE	2.50	0.44
1:B:1262:LYS:NZ	7:B:2155:HOH:O	2.27	0.44
1:C:761:GLU:OE2	1:D:798:ARG:NH2	2.48	0.44
1:C:767:ILE:HD12	1:C:792:ILE:CD1	2.47	0.44
1:C:1169:ILE:HG12	1:C:1282:ALA:HB1	2.00	0.44
1:D:231:ASN:O	1:D:231:ASN:CG	2.61	0.44
1:A:387:ILE:CG2	1:A:388:GLN:N	2.81	0.44
1:A:576:LEU:HA	1:A:582:ARG:NH2	2.32	0.44
1:A:791:ARG:NH2	7:A:2135:HOH:O	2.50	0.44
1:A:1067:HIS:HE1	1:B:764:GLU:OE2	2.00	0.44
1:B:319:LEU:O	1:B:323:VAL:HG13	2.17	0.44
1:B:836:ASP:O	1:B:840:ILE:HG13	2.17	0.44
1:B:880:GLU:N	1:B:880:GLU:CD	2.75	0.44
1:C:1131:SER:HB2	1:D:1137:TYR:CG	2.53	0.44
1:D:767:ILE:HD12	1:D:792:ILE:CD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:838:MET:HE2	1:D:838:MET:HB3	1.86	0.44
1:A:1137:TYR:CG	1:B:1131:SER:HB2	2.52	0.44
1:B:210:LEU:O	1:B:212:PRO:HD3	2.17	0.44
1:B:624:ILE:HD11	1:B:664:VAL:HG13	1.98	0.44
1:C:111:LYS:HB3	7:C:2020:HOH:O	2.17	0.44
1:C:485:TRP:CD1	1:C:485:TRP:O	2.71	0.44
1:C:1023:ALA:HB3	1:C:1076:VAL:CG1	2.48	0.44
1:D:361:SER:O	1:D:362:ARG:C	2.60	0.44
1:D:746:HIS:HA	1:D:916:PHE:CE2	2.53	0.44
1:D:798:ARG:HD3	7:D:2028:HOH:O	2.17	0.44
1:D:1169:ILE:HG12	1:D:1282:ALA:HB1	2.00	0.44
1:A:115:THR:CG2	1:A:592:HIS:ND1	2.81	0.44
1:A:217:ILE:O	1:A:218:PHE:C	2.60	0.44
1:A:703:VAL:HG23	1:A:906:CYS:SG	2.57	0.44
1:A:727:ALA:HB2	1:A:898:ASN:HD22	1.81	0.44
1:B:798:ARG:HG2	1:B:798:ARG:NH1	2.33	0.44
1:D:91:THR:N	7:D:2004:HOH:O	2.31	0.44
1:D:360:ILE:HG13	6:D:3005:FAD:N3A	2.32	0.44
1:D:362:ARG:HB3	7:D:2064:HOH:O	2.16	0.44
1:B:429:ARG:NH2	1:B:437:ALA:O	2.51	0.44
1:B:844:ARG:NH1	1:B:916:PHE:HB3	2.33	0.44
1:B:997:PHE:CD1	1:B:997:PHE:C	2.96	0.44
1:D:52:CYS:C	1:D:54:ALA:H	2.26	0.44
1:D:691:ILE:HD11	1:D:693:TYR:CE1	2.53	0.44
1:B:35:ARG:HD2	1:B:43:THR:O	2.18	0.43
1:B:44:LYS:HE2	1:B:44:LYS:HB3	1.72	0.43
1:C:659:TYR:CE2	1:C:819:VAL:HG21	2.53	0.43
1:C:879:SER:O	1:C:882:VAL:HB	2.17	0.43
1:D:235:THR:HA	1:D:243:TRP:O	2.18	0.43
1:D:624:ILE:HD11	1:D:664:VAL:HG13	2.00	0.43
1:D:1103:MET:HE1	1:D:1118:TRP:HZ3	1.83	0.43
1:D:1252:THR:HG21	7:D:2125:HOH:O	2.18	0.43
1:A:235:THR:HA	1:A:243:TRP:O	2.19	0.43
1:A:319:LEU:O	1:A:323:VAL:HG13	2.17	0.43
1:A:333:ILE:HA	1:A:425:VAL:HG21	2.00	0.43
1:B:1085:SER:OG	1:B:1266:GLU:HG3	2.19	0.43
1:C:880:GLU:N	1:C:880:GLU:CD	2.76	0.43
1:D:72:PHE:C	7:D:2013:HOH:O	2.52	0.43
1:D:498:CYS:SG	1:D:1318:LEU:CB	3.07	0.43
1:A:1334:VAL:O	1:A:1334:VAL:HG12	2.17	0.43
1:B:871:ASN:HD21	1:B:908:THR:HG21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:890:LEU:HD12	1:B:890:LEU:C	2.43	0.43
1:C:51:ASP:OD1	1:C:51:ASP:O	2.36	0.43
1:C:317:ASN:ND2	7:C:2053:HOH:O	2.51	0.43
1:C:333:ILE:HA	1:C:425:VAL:HG21	2.00	0.43
1:A:1230:HIS:N	1:A:1230:HIS:CD2	2.86	0.43
1:B:66:SER:O	1:B:67:LYS:CB	2.66	0.43
1:C:703:VAL:HG23	1:C:906:CYS:SG	2.58	0.43
1:C:746:HIS:HA	1:C:916:PHE:CE2	2.53	0.43
1:C:758:PRO:C	1:C:760:GLY:H	2.27	0.43
1:C:767:ILE:CD1	1:C:792:ILE:HD12	2.49	0.43
1:D:429:ARG:NH2	1:D:437:ALA:O	2.52	0.43
1:D:1021:GLN:HA	1:D:1138:PHE:O	2.18	0.43
1:B:46:GLY:O	1:B:834:ARG:NE	2.36	0.43
1:B:844:ARG:HG2	1:B:923:GLN:NE2	2.33	0.43
1:B:1138:PHE:CE2	1:B:1140:GLY:HA2	2.53	0.43
1:C:709:TYR:O	1:C:710:GLU:C	2.59	0.43
1:C:969:LEU:HA	1:C:1160:PHE:HB3	2.00	0.43
1:C:1334:VAL:O	1:C:1334:VAL:HG12	2.18	0.43
1:D:709:TYR:O	1:D:710:GLU:C	2.61	0.43
1:D:997:PHE:C	1:D:997:PHE:CD1	2.96	0.43
1:A:147:LEU:C	1:A:149:GLY:H	2.26	0.43
1:A:1185:MET:SD	1:A:1267:ALA:HB1	2.58	0.43
1:A:1203:ALA:O	1:A:1269:THR:HA	2.19	0.43
1:B:727:ALA:HB2	1:B:898:ASN:HD22	1.82	0.43
1:B:758:PRO:C	1:B:760:GLY:H	2.26	0.43
1:C:435:GLN:HG2	1:C:436:ASN:N	2.34	0.43
1:C:1025:LEU:HD13	1:C:1135:THR:CG2	2.49	0.43
1:D:275:MET:CG	1:D:282:TYR:CE2	3.01	0.43
1:D:1185:MET:SD	1:D:1267:ALA:HB1	2.59	0.43
1:D:1334:VAL:O	1:D:1334:VAL:HG12	2.19	0.43
1:A:44:LYS:HB3	1:A:44:LYS:HE2	1.72	0.43
1:A:51:ASP:OD1	1:A:51:ASP:O	2.37	0.43
1:A:614:VAL:HG12	1:A:673:ALA:CB	2.48	0.43
1:A:879:SER:HB3	1:A:905:VAL:HG11	2.00	0.43
1:A:1332:ILE:HG13	1:A:1332:ILE:O	2.18	0.43
1:B:42:GLY:O	1:B:44:LYS:HE3	2.19	0.43
1:D:42:GLY:O	1:D:44:LYS:HE3	2.18	0.43
1:D:319:LEU:HB3	1:D:338:LEU:HD23	2.01	0.43
1:D:712:PHE:CB	1:D:904:ARG:NH1	2.82	0.43
1:D:992:PHE:CE1	1:D:1001:ARG:HG3	2.53	0.43
1:A:147:LEU:O	1:A:148:GLY:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:ARG:NH2	1:A:437:ALA:O	2.51	0.43
1:A:600:CYS:O	1:A:603:MET:HG3	2.18	0.43
1:A:792:ILE:O	1:A:792:ILE:HG12	2.19	0.43
1:A:1243:GLU:HG2	1:A:1245:HIS:HE2	1.84	0.43
1:B:319:LEU:HD12	1:B:319:LEU:HA	1.76	0.43
1:C:33:TYR:O	1:C:37:VAL:CG1	2.67	0.43
1:C:461:ILE:HB	1:C:473:ALA:HB3	2.00	0.43
1:D:84:LEU:O	1:D:85:HIS:C	2.62	0.43
1:D:92:VAL:HG12	1:D:93:GLU:OE1	2.19	0.43
1:D:357:GLY:CA	6:D:3005:FAD:H51A	2.47	0.43
1:D:586:HIS:O	1:D:589:GLY:N	2.40	0.43
1:D:866:ILE:CD1	1:D:927:VAL:HG11	2.48	0.43
1:D:1097:ASN:ND2	1:D:1137:TYR:H	2.09	0.43
1:D:1313:ASP:HB2	7:D:2155:HOH:O	2.18	0.43
1:A:570:VAL:HG11	1:A:582:ARG:NH1	2.34	0.43
1:B:231:ASN:O	1:B:231:ASN:CG	2.62	0.43
1:B:232:THR:H	1:B:290:ARG:HH22	1.66	0.43
1:B:600:CYS:O	1:B:603:MET:HG3	2.18	0.43
1:B:754:VAL:HG22	1:B:755:ARG:N	2.33	0.43
1:B:792:ILE:HG12	1:B:792:ILE:O	2.19	0.43
1:B:984:ASN:ND2	7:B:2135:HOH:O	2.47	0.43
1:C:66:SER:O	1:C:67:LYS:CB	2.66	0.43
1:C:92:VAL:HG12	1:C:93:GLU:OE1	2.19	0.43
1:C:506:ALA:CB	1:C:512:GLU:CG	2.97	0.43
1:C:624:ILE:HD11	1:C:664:VAL:HG13	2.01	0.43
1:D:1332:ILE:HG13	1:D:1332:ILE:O	2.19	0.43
1:A:33:TYR:CE1	1:A:37:VAL:HG11	2.54	0.43
1:A:361:SER:O	1:A:362:ARG:C	2.61	0.43
1:A:930:THR:O	1:A:930:THR:HG22	2.18	0.43
1:A:1202:GLY:O	1:A:1205:VAL:N	2.50	0.43
1:B:25:ASP:HB3	1:B:28:VAL:HG12	2.01	0.43
1:B:235:THR:HA	1:B:243:TRP:O	2.19	0.43
1:B:518:LEU:HD21	1:B:1173:THR:HA	2.00	0.43
1:B:624:ILE:HB	1:B:662:ASP:O	2.18	0.43
1:B:930:THR:O	1:B:930:THR:HG22	2.18	0.43
1:B:1025:LEU:HD13	1:B:1135:THR:CG2	2.49	0.43
1:B:1220:PRO:HA	1:B:1332:ILE:CD1	2.48	0.43
1:B:1308:ARG:HG3	1:B:1309:MET:HE2	2.01	0.43
1:C:33:TYR:CE1	1:C:37:VAL:HG11	2.54	0.43
1:C:1243:GLU:HG2	1:C:1245:HIS:NE2	2.34	0.43
1:C:1308:ARG:HG3	1:C:1309:MET:HE2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:333:ILE:HA	1:D:425:VAL:HG21	2.01	0.43
1:D:395:HIS:C	1:D:397:LEU:N	2.76	0.43
1:D:652:GLY:C	7:D:2095:HOH:O	2.61	0.43
1:D:956:ASP:CG	1:D:957:ARG:H	2.25	0.43
1:D:1308:ARG:HG3	1:D:1309:MET:HE2	2.01	0.43
1:A:702:THR:O	1:A:705:ASP:HB2	2.19	0.42
1:A:969:LEU:HA	1:A:1160:PHE:HB3	2.00	0.42
1:B:333:ILE:HA	1:B:425:VAL:HG21	2.00	0.42
1:B:969:LEU:N	7:B:2131:HOH:O	2.52	0.42
1:B:992:PHE:CE1	1:B:1001:ARG:HG3	2.54	0.42
1:B:1036:VAL:HG12	1:B:1037:ALA:N	2.34	0.42
1:C:893:ALA:HB1	1:C:969:LEU:HD11	1.99	0.42
1:D:712:PHE:HB3	1:D:904:ARG:NH1	2.34	0.42
1:D:879:SER:O	1:D:882:VAL:HB	2.19	0.42
1:D:1107:GLU:HB3	1:D:1108:PRO:CD	2.49	0.42
1:D:1271:LEU:HA	1:D:1271:LEU:HD23	1.78	0.42
1:A:33:TYR:O	1:A:37:VAL:CG1	2.68	0.42
1:A:47:CYS:SG	1:A:1229:PRO:HG2	2.59	0.42
1:A:758:PRO:C	1:A:760:GLY:H	2.26	0.42
1:A:893:ALA:HB1	1:A:969:LEU:HD11	2.01	0.42
1:B:315:VAL:O	1:B:319:LEU:HB2	2.19	0.42
1:C:72:PHE:HD2	1:C:351:ASN:HB3	1.84	0.42
1:C:210:LEU:O	1:C:212:PRO:HD3	2.20	0.42
1:C:326:LEU:HG	1:C:327:PRO:HD2	2.01	0.42
1:C:387:ILE:H	1:C:387:ILE:CD1	2.30	0.42
1:D:279:ASP:CG	1:D:687:LYS:HD3	2.44	0.42
1:D:315:VAL:O	1:D:319:LEU:HB2	2.19	0.42
1:D:1036:VAL:HG12	1:D:1037:ALA:N	2.32	0.42
1:A:97:SER:HB2	7:A:2022:HOH:O	2.20	0.42
1:A:356:GLY:CA	7:A:2058:HOH:O	2.67	0.42
1:A:717:ARG:HD3	1:A:884:GLU:HG2	2.01	0.42
1:A:992:PHE:CE1	1:A:1001:ARG:HG3	2.55	0.42
1:A:1252:THR:HG23	1:A:1253:PRO:HD2	2.02	0.42
1:C:35:ARG:HD2	1:C:43:THR:O	2.18	0.42
1:C:868:LEU:HD12	1:C:887:LEU:CD2	2.48	0.42
1:D:222:LEU:HD23	1:D:222:LEU:HA	1.79	0.42
1:D:614:VAL:HG12	1:D:673:ALA:CB	2.49	0.42
1:D:792:ILE:O	1:D:792:ILE:HG12	2.18	0.42
1:D:893:ALA:HB1	1:D:969:LEU:HD11	2.01	0.42
1:D:973:TRP:O	1:D:977:VAL:HG23	2.19	0.42
1:A:391:PRO:O	7:A:2069:HOH:O	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:LEU:HD12	1:A:887:LEU:CD2	2.49	0.42
1:B:632:ALA:O	1:B:633:LEU:C	2.61	0.42
1:C:844:ARG:HG2	1:C:923:GLN:NE2	2.34	0.42
1:C:1012:VAL:O	1:C:1156:PRO:HD2	2.19	0.42
1:D:702:THR:O	1:D:705:ASP:HB2	2.19	0.42
1:D:890:LEU:HD21	1:D:901:VAL:CG2	2.38	0.42
1:D:1219:SER:OG	1:D:1223:VAL:CG1	2.63	0.42
1:A:138:PRO:O	1:A:168:CYS:HB3	2.19	0.42
1:A:746:HIS:HA	1:A:916:PHE:CE2	2.53	0.42
1:A:890:LEU:HD12	1:A:891:GLU:N	2.34	0.42
1:A:1021:GLN:HA	1:A:1138:PHE:O	2.20	0.42
1:B:103:HIS:CG	1:B:104:PRO:HD2	2.55	0.42
1:B:395:HIS:C	1:B:397:LEU:N	2.76	0.42
1:B:463:TYR:O	1:B:470:VAL:HG12	2.19	0.42
1:B:879:SER:O	1:B:882:VAL:HB	2.19	0.42
1:C:25:ASP:HA	1:C:26:PRO:HD3	1.88	0.42
1:C:1006:ILE:HD11	1:C:1271:LEU:HA	2.01	0.42
1:C:1036:VAL:HG12	1:C:1037:ALA:N	2.34	0.42
1:C:1103:MET:HE1	1:C:1118:TRP:HZ3	1.85	0.42
1:D:35:ARG:HD2	1:D:43:THR:O	2.20	0.42
1:D:50:GLY:CA	3:D:3002:FES:S2	3.08	0.42
1:D:844:ARG:HG2	1:D:923:GLN:NE2	2.34	0.42
1:D:880:GLU:O	1:D:884:GLU:HG3	2.20	0.42
1:A:513:GLU:HG2	1:A:514:TYR:H	1.83	0.42
1:A:764:GLU:OE2	1:B:1067:HIS:HE1	2.02	0.42
1:A:1027:GLN:HG3	1:B:1077:PRO:CG	2.45	0.42
1:A:1220:PRO:HA	1:A:1332:ILE:CD1	2.48	0.42
1:B:1219:SER:HG	1:B:1223:VAL:HG12	1.85	0.42
1:C:115:THR:HG23	1:C:592:HIS:ND1	2.35	0.42
1:C:132:LEU:HD12	1:C:132:LEU:HA	1.86	0.42
1:C:315:VAL:O	1:C:319:LEU:HB2	2.20	0.42
1:C:591:LYS:HD2	1:D:761:GLU:HG3	2.02	0.42
1:D:72:PHE:HD2	1:D:351:ASN:HB3	1.84	0.42
1:D:269:THR:OG1	6:D:3005:FAD:O2P	2.38	0.42
1:D:836:ASP:O	1:D:840:ILE:HG13	2.19	0.42
1:D:1220:PRO:HA	1:D:1332:ILE:CD1	2.49	0.42
1:A:627:LEU:HD13	1:A:627:LEU:C	2.45	0.42
1:B:472:SER:C	1:B:474:ASP:N	2.77	0.42
1:B:969:LEU:HA	1:B:1160:PHE:HB3	2.01	0.42
1:C:720:GLU:O	1:C:721:GLN:HG2	2.20	0.42
1:D:264:LEU:O	6:D:3005:FAD:C8A	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:844:ARG:NH1	1:D:916:PHE:HB3	2.34	0.42
1:A:58:MET:HG3	7:A:2015:HOH:O	2.15	0.42
1:A:767:ILE:CD1	1:A:792:ILE:HD12	2.49	0.42
1:A:997:PHE:CD1	1:A:997:PHE:C	2.97	0.42
1:A:1085:SER:OG	1:A:1266:GLU:HG3	2.19	0.42
1:B:148:GLY:C	7:B:2029:HOH:O	2.62	0.42
1:B:387:ILE:CG2	1:B:388:GLN:N	2.82	0.42
1:B:485:TRP:O	1:B:485:TRP:CD1	2.72	0.42
1:B:883:ILE:HD12	1:B:883:ILE:HA	1.90	0.42
1:B:1202:GLY:O	1:B:1205:VAL:N	2.52	0.42
1:C:199:THR:HG21	7:C:2028:HOH:O	2.19	0.42
1:C:788:PRO:HG2	1:C:791:ARG:HH12	1.82	0.42
1:C:997:PHE:CD1	1:C:997:PHE:C	2.98	0.42
1:D:156:GLY:O	1:D:157:TYR:HB2	2.20	0.42
1:A:259:HIS:NE2	7:A:2050:HOH:O	2.10	0.42
1:A:890:LEU:HD21	1:A:901:VAL:CG2	2.39	0.42
1:A:980:SER:HB2	1:A:985:ARG:NH2	2.35	0.42
1:A:1043:LEU:HG	1:A:1045:GLN:HE22	1.84	0.42
1:B:311:SER:O	1:B:315:VAL:HG23	2.19	0.42
1:B:435:GLN:NE2	7:B:2029:HOH:O	2.38	0.42
1:B:866:ILE:CD1	1:B:927:VAL:HG11	2.50	0.42
1:B:1107:GLU:HB3	1:B:1108:PRO:CD	2.49	0.42
1:B:1243:GLU:HG2	1:B:1245:HIS:HE2	1.85	0.42
1:C:147:LEU:C	1:C:149:GLY:H	2.28	0.42
1:C:463:TYR:O	1:C:470:VAL:HG12	2.20	0.42
1:C:1062:PRO:HD2	1:C:1065:TYR:CD1	2.55	0.42
1:D:868:LEU:HD11	1:D:890:LEU:CD2	2.49	0.42
1:A:25:ASP:HB3	1:A:28:VAL:HG12	2.02	0.42
1:A:315:VAL:O	1:A:319:LEU:HB2	2.20	0.42
1:A:1243:GLU:HG2	1:A:1245:HIS:NE2	2.35	0.42
1:B:52:CYS:C	1:B:54:ALA:H	2.27	0.42
1:B:973:TRP:O	1:B:977:VAL:HG23	2.20	0.42
1:C:358:HIS:CA	6:C:3005:FAD:O4'	2.67	0.42
1:D:758:PRO:C	1:D:760:GLY:H	2.27	0.42
1:D:838:MET:SD	1:D:1228:GLY:N	2.93	0.42
1:D:894:TYR:CD1	1:D:894:TYR:N	2.88	0.42
1:D:1230:HIS:N	1:D:1230:HIS:CD2	2.88	0.42
1:A:51:ASP:HB3	1:A:1229:PRO:HB2	2.02	0.41
1:A:879:SER:O	1:A:882:VAL:HB	2.20	0.41
1:A:890:LEU:HD12	1:A:890:LEU:C	2.45	0.41
1:A:1055:ALA:CB	1:A:1066:ILE:HD13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:339:LYS:HA	1:C:342:LYS:HE3	2.01	0.41
1:C:724:VAL:HG22	1:C:728:PHE:CE2	2.55	0.41
1:D:374:ILE:HG13	1:D:374:ILE:O	2.20	0.41
1:A:775:ALA:O	1:A:778:GLN:HB3	2.20	0.41
1:A:880:GLU:CD	1:A:880:GLU:H	2.28	0.41
7:A:2162:HOH:O	1:B:759:LYS:CE	2.63	0.41
1:B:319:LEU:HB3	1:B:338:LEU:HD23	2.03	0.41
1:B:360:ILE:HG21	6:B:3005:FAD:H1B	2.01	0.41
1:C:374:ILE:HG13	1:C:374:ILE:O	2.21	0.41
1:C:1018:PHE:HB3	1:D:1127:VAL:O	2.19	0.41
1:D:485:TRP:O	1:D:485:TRP:CD1	2.73	0.41
1:D:624:ILE:HB	1:D:662:ASP:O	2.20	0.41
1:D:717:ARG:HD3	1:D:884:GLU:HG2	2.01	0.41
1:D:1243:GLU:HG2	1:D:1245:HIS:HE2	1.85	0.41
1:D:1243:GLU:HG2	1:D:1245:HIS:NE2	2.35	0.41
1:A:84:LEU:O	1:A:85:HIS:C	2.62	0.41
1:A:1105:ARG:NH1	1:A:1131:SER:O	2.53	0.41
1:B:147:LEU:O	1:B:148:GLY:C	2.61	0.41
1:B:1243:GLU:HG2	1:B:1245:HIS:NE2	2.35	0.41
1:B:1332:ILE:O	1:B:1332:ILE:HG13	2.20	0.41
1:C:211:ASP:OD2	7:C:2032:HOH:O	2.21	0.41
1:C:218:PHE:HA	1:C:219:PRO:HD3	1.92	0.41
1:C:1078:ASN:OD1	1:D:1029:TYR:HA	2.20	0.41
1:D:356:GLY:N	7:D:2057:HOH:O	2.49	0.41
1:D:868:LEU:O	1:D:903:GLY:HA2	2.21	0.41
1:A:755:ARG:HG2	1:A:829:ARG:HG3	2.02	0.41
1:C:147:LEU:O	1:C:148:GLY:C	2.64	0.41
1:C:755:ARG:HG2	1:C:829:ARG:HG3	2.01	0.41
1:C:890:LEU:HD12	1:C:890:LEU:C	2.45	0.41
1:D:132:LEU:HD12	1:D:132:LEU:HA	1.88	0.41
1:D:210:LEU:O	1:D:212:PRO:HD3	2.20	0.41
1:A:395:HIS:C	1:A:397:LEU:N	2.74	0.41
1:A:1006:ILE:HD11	1:A:1271:LEU:HA	2.01	0.41
1:B:349:ILE:HD13	1:B:349:ILE:HA	1.82	0.41
1:B:456:ILE:HG13	1:B:483:ARG:O	2.20	0.41
1:B:513:GLU:HG2	1:B:514:TYR:H	1.84	0.41
1:B:704:GLN:HE21	1:B:704:GLN:N	2.07	0.41
1:B:868:LEU:HD12	1:B:887:LEU:CD2	2.49	0.41
1:B:890:LEU:HD21	1:B:901:VAL:CG2	2.40	0.41
1:B:980:SER:HB2	1:B:985:ARG:NH2	2.36	0.41
1:B:1230:HIS:N	1:B:1230:HIS:CD2	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:CYS:C	1:C:54:ALA:H	2.29	0.41
1:C:138:PRO:O	1:C:168:CYS:HB3	2.20	0.41
1:C:426:SER:HB2	1:C:526:PHE:CD1	2.56	0.41
1:C:762:ASP:OD2	1:D:591:LYS:NZ	2.52	0.41
1:C:816:VAL:O	1:C:819:VAL:HG22	2.21	0.41
1:C:838:MET:HE2	1:C:838:MET:HB3	1.86	0.41
1:C:1055:ALA:CB	1:C:1066:ILE:HD13	2.50	0.41
1:D:339:LYS:HA	1:D:342:LYS:HE3	2.02	0.41
1:D:788:PRO:HG2	1:D:791:ARG:HH12	1.85	0.41
1:D:1055:ALA:CB	1:D:1066:ILE:HD13	2.49	0.41
1:D:1086:THR:O	1:D:1087:GLY:C	2.64	0.41
1:D:1252:THR:HG23	1:D:1253:PRO:HD2	2.01	0.41
1:A:366:SER:HA	6:A:3005:FAD:O2	2.20	0.41
1:A:374:ILE:O	1:A:374:ILE:HG13	2.20	0.41
1:A:615:VAL:HG13	1:A:672:CYS:SG	2.61	0.41
1:A:1036:VAL:HG12	1:A:1037:ALA:N	2.34	0.41
1:B:51:ASP:OD1	1:B:51:ASP:O	2.39	0.41
1:B:415:PHE:HD1	1:B:416:VAL:N	2.18	0.41
1:B:992:PHE:CE1	1:B:996:ARG:HG3	2.54	0.41
1:B:1059:LEU:HA	1:B:1103:MET:SD	2.60	0.41
1:B:1316:THR:O	1:B:1316:THR:HG23	2.21	0.41
1:C:1107:GLU:HB3	1:C:1108:PRO:CD	2.51	0.41
1:C:1230:HIS:N	1:C:1230:HIS:CD2	2.89	0.41
1:D:52:CYS:O	1:D:54:ALA:N	2.54	0.41
1:D:463:TYR:O	1:D:470:VAL:HG12	2.21	0.41
1:D:890:LEU:HD12	1:D:890:LEU:C	2.46	0.41
1:D:1035:LEU:CD1	7:D:2134:HOH:O	2.68	0.41
1:D:1294:PRO:O	1:D:1295:ILE:C	2.63	0.41
1:A:373:GLY:HA2	1:A:392:LEU:O	2.21	0.41
1:B:374:ILE:HG13	1:B:374:ILE:O	2.21	0.41
1:B:717:ARG:HD3	1:B:884:GLU:HG2	2.03	0.41
1:C:992:PHE:CE1	1:C:1001:ARG:HG3	2.56	0.41
1:D:90:THR:N	7:D:2012:HOH:O	2.46	0.41
1:D:128:ILE:O	1:D:129:TYR:C	2.64	0.41
1:D:308:THR:HG21	6:D:3005:FAD:H61A	1.82	0.41
1:D:426:SER:HB2	1:D:526:PHE:CD1	2.55	0.41
1:D:1107:GLU:N	1:D:1108:PRO:HD2	2.36	0.41
1:A:114:GLY:CA	1:A:159:PRO:HB2	2.48	0.41
1:A:1161:GLY:O	1:A:1162:ALA:HB2	2.21	0.41
1:B:422:TRP:CG	1:B:451:GLU:HA	2.56	0.41
1:B:448:VAL:O	1:B:457:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1062:PRO:HD2	1:B:1065:TYR:CD1	2.56	0.41
1:B:1161:GLY:HA3	1:B:1185:MET:CE	2.48	0.41
1:C:473:ALA:O	1:C:474:ASP:C	2.62	0.41
1:C:1005:ILE:HG23	1:C:1005:ILE:O	2.21	0.41
1:D:264:LEU:HD22	1:D:264:LEU:N	2.35	0.41
1:D:826:ARG:HE	1:D:826:ARG:HB3	1.64	0.41
1:A:103:HIS:CG	1:A:104:PRO:HD2	2.55	0.41
1:A:320:SER:HA	1:A:323:VAL:HG22	2.03	0.41
1:A:716:GLU:HA	1:A:904:ARG:HG3	2.02	0.41
1:A:826:ARG:HE	1:A:826:ARG:HB3	1.65	0.41
1:A:834:ARG:O	1:A:838:MET:HG3	2.20	0.41
1:A:867:GLN:CD	1:A:869:TYR:HH	2.14	0.41
1:A:1107:GLU:HB3	1:A:1108:PRO:CD	2.50	0.41
1:A:1219:SER:O	1:A:1220:PRO:C	2.63	0.41
1:B:33:TYR:CE1	1:B:37:VAL:HG11	2.56	0.41
1:B:138:PRO:O	1:B:168:CYS:HB3	2.21	0.41
1:B:218:PHE:HA	1:B:219:PRO:HD3	1.94	0.41
1:B:838:MET:HE2	1:B:838:MET:HB3	1.86	0.41
1:B:868:LEU:O	1:B:903:GLY:HA2	2.21	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.78	0.41
1:C:269:THR:OG1	6:C:3005:FAD:O2P	2.31	0.41
1:C:297:VAL:O	1:C:297:VAL:HG13	2.21	0.41
1:C:353:ALA:HB1	6:C:3005:FAD:H4'	2.02	0.41
1:C:387:ILE:CG2	1:C:388:GLN:N	2.84	0.41
1:C:643:THR:OG1	7:C:2084:HOH:O	1.92	0.41
1:C:834:ARG:O	1:C:838:MET:HG3	2.21	0.41
1:C:980:SER:HB2	1:C:985:ARG:NH2	2.35	0.41
1:C:1078:ASN:ND2	1:D:1028:ILE:O	2.49	0.41
1:D:51:ASP:OD1	1:D:51:ASP:O	2.39	0.41
1:D:124:MET:O	1:D:125:VAL:C	2.62	0.41
1:D:291:ILE:N	1:D:291:ILE:CD1	2.84	0.41
1:D:868:LEU:HD12	1:D:887:LEU:CD2	2.50	0.41
1:D:969:LEU:HA	1:D:1160:PHE:HB3	2.02	0.41
1:D:1085:SER:OG	1:D:1266:GLU:HG3	2.21	0.41
1:A:199:THR:CA	7:A:2037:HOH:O	2.68	0.41
1:A:485:TRP:CD1	1:A:485:TRP:O	2.74	0.41
1:A:866:ILE:CD1	1:A:927:VAL:HG11	2.51	0.41
1:A:951:MET:N	7:A:2143:HOH:O	1.87	0.41
1:A:1256:LYS:NZ	7:A:2174:HOH:O	2.30	0.41
1:B:426:SER:HB2	1:B:526:PHE:CD1	2.56	0.41
1:B:767:ILE:HD12	1:B:792:ILE:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:767:ILE:HD12	1:B:792:ILE:CD1	2.51	0.41
1:B:830:PHE:CZ	1:B:832:LEU:HD11	2.56	0.41
1:B:894:TYR:CD1	1:B:894:TYR:N	2.89	0.41
1:B:1271:LEU:HA	1:B:1271:LEU:HD23	1.78	0.41
1:C:584:ILE:HG21	1:C:1063:MET:HE1	2.01	0.41
1:D:275:MET:CG	1:D:282:TYR:HE2	2.34	0.41
1:D:716:GLU:HA	1:D:904:ARG:HG3	2.02	0.41
1:D:1203:ALA:O	1:D:1269:THR:HA	2.21	0.41
1:A:124:MET:O	1:A:125:VAL:C	2.64	0.40
1:A:210:LEU:O	1:A:212:PRO:HD3	2.21	0.40
1:A:279:ASP:CG	1:A:687:LYS:HD3	2.47	0.40
1:A:339:LYS:HA	1:A:342:LYS:HE3	2.02	0.40
1:A:426:SER:HB2	1:A:526:PHE:CD1	2.56	0.40
1:A:624:ILE:HD11	1:A:664:VAL:HG13	2.02	0.40
1:A:839:LEU:HD23	1:A:839:LEU:HA	1.86	0.40
1:A:1055:ALA:HB3	1:A:1066:ILE:HD13	2.02	0.40
1:B:390:ILE:C	7:B:2055:HOH:O	2.63	0.40
1:B:570:VAL:HG11	1:B:582:ARG:NH1	2.36	0.40
1:B:1334:VAL:O	1:B:1334:VAL:HG12	2.21	0.40
1:C:154:CYS:O	1:C:1202:GLY:HA3	2.20	0.40
1:C:235:THR:HA	1:C:243:TRP:O	2.20	0.40
1:C:1107:GLU:N	1:C:1108:PRO:HD2	2.36	0.40
1:D:116:GLN:HB3	1:D:1044:GLY:O	2.21	0.40
1:D:242:THR:O	1:D:242:THR:HG22	2.20	0.40
1:D:354:SER:HB2	7:D:2057:HOH:O	2.20	0.40
1:D:448:VAL:O	1:D:457:THR:HB	2.22	0.40
1:D:720:GLU:O	1:D:721:GLN:HG2	2.21	0.40
1:A:203:GLU:O	1:A:206:GLU:HG2	2.21	0.40
1:B:880:GLU:CD	1:B:880:GLU:H	2.29	0.40
1:C:358:HIS:HB2	6:C:3005:FAD:O4'	2.21	0.40
1:C:505:MET:SD	1:C:512:GLU:HG3	2.61	0.40
1:C:866:ILE:CD1	1:C:927:VAL:HG11	2.51	0.40
1:C:967:THR:N	7:C:2113:HOH:O	2.53	0.40
1:C:1041:VAL:O	1:C:1047:ILE:HD11	2.21	0.40
1:C:1111:LYS:HA	1:C:1111:LYS:HD3	1.68	0.40
1:D:25:ASP:HA	1:D:26:PRO:HD3	1.91	0.40
1:D:90:THR:CA	7:D:2012:HOH:O	2.68	0.40
1:A:92:VAL:HG12	1:A:93:GLU:OE1	2.22	0.40
1:A:883:ILE:HD12	1:A:883:ILE:HA	1.93	0.40
1:A:894:TYR:CD1	1:A:894:TYR:N	2.89	0.40
1:B:72:PHE:HD2	1:B:351:ASN:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:THR:O	1:B:317:ASN:ND2	2.54	0.40
1:B:373:GLY:HA2	1:B:392:LEU:O	2.22	0.40
1:B:703:VAL:HG13	1:B:704:GLN:HE22	1.84	0.40
1:B:1203:ALA:O	1:B:1269:THR:HA	2.22	0.40
1:C:448:VAL:O	1:C:457:THR:HB	2.22	0.40
1:C:600:CYS:O	1:C:603:MET:HG3	2.21	0.40
1:C:775:ALA:O	1:C:778:GLN:HB3	2.21	0.40
1:C:956:ASP:CG	1:C:957:ARG:H	2.26	0.40
1:D:160:ILE:O	1:D:161:VAL:C	2.64	0.40
1:A:408:GLU:H	1:A:408:GLU:HG3	1.57	0.40
1:A:764:GLU:HA	1:A:791:ARG:O	2.22	0.40
1:B:465:GLY:O	1:B:515:ARG:HD2	2.21	0.40
1:B:716:GLU:HA	1:B:904:ARG:HG3	2.02	0.40
1:B:739:VAL:CG1	1:B:930:THR:HG21	2.48	0.40
1:B:838:MET:SD	1:B:1228:GLY:N	2.94	0.40
1:B:956:ASP:CG	1:B:957:ARG:H	2.26	0.40
1:B:1014:PHE:CG	1:B:1019:TYR:HB3	2.57	0.40
1:C:493:ALA:O	1:C:497:ILE:HG12	2.21	0.40
1:C:624:ILE:HB	1:C:662:ASP:O	2.22	0.40
1:C:655:GLU:O	1:C:655:GLU:CG	2.70	0.40
1:C:973:TRP:O	1:C:977:VAL:HG23	2.21	0.40
1:C:1105:ARG:NH1	1:C:1131:SER:O	2.54	0.40
1:D:47:CYS:CB	1:D:1229:PRO:HG2	2.52	0.40
1:D:311:SER:O	1:D:315:VAL:HG23	2.21	0.40
1:D:347:GLN:O	1:D:348:GLN:C	2.65	0.40
1:D:910:LEU:HD23	7:D:2100:HOH:O	2.21	0.40
1:D:1193:PRO:O	1:D:1197:ILE:HG12	2.22	0.40
1:A:1308:ARG:HG3	1:A:1309:MET:HE2	2.02	0.40
1:C:717:ARG:HD3	1:C:884:GLU:HG2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1221/1335 (92%)	1123 (92%)	89 (7%)	9 (1%)	18	25
1	B	1238/1335 (93%)	1137 (92%)	93 (8%)	8 (1%)	21	29
1	C	1210/1335 (91%)	1111 (92%)	88 (7%)	11 (1%)	14	20
1	D	1231/1335 (92%)	1120 (91%)	104 (8%)	7 (1%)	21	29
All	All	4900/5340 (92%)	4491 (92%)	374 (8%)	35 (1%)	18	25

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	ALA
1	B	762	ASP
1	C	398	ALA
1	C	474	ASP
1	A	762	ASP
1	B	451	GLU
1	B	474	ASP
1	C	762	ASP
1	D	762	ASP
1	A	662	ASP
1	B	148	GLY
1	B	662	ASP
1	C	662	ASP
1	D	662	ASP
1	A	632	ALA
1	A	1188	SER
1	B	1188	SER
1	C	632	ALA
1	D	1188	SER
1	A	362	ARG
1	B	632	ALA
1	C	362	ARG
1	C	1188	SER
1	D	148	GLY
1	D	632	ALA
1	A	1318	LEU
1	A	1320	PRO
1	C	507	ALA
1	D	53	GLY
1	B	796	VAL
1	C	1295	ILE
1	D	796	VAL
1	A	148	GLY

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Mol	Chain	Res	Type
1	C	148	GLY
1	C	796	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	958/1129 (85%)	856 (89%)	102 (11%)	6	7
1	B	988/1129 (88%)	879 (89%)	109 (11%)	6	6
1	C	948/1129 (84%)	853 (90%)	95 (10%)	7	9
1	D	941/1129 (83%)	845 (90%)	96 (10%)	7	8
All	All	3835/4516 (85%)	3433 (90%)	402 (10%)	6	8

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	11	ILE
1	A	20	THR
1	A	28	VAL
1	A	36	LYS
1	A	43	THR
1	A	44	LYS
1	A	59	ILE
1	A	66	SER
1	A	97	SER
1	A	115	THR
1	A	127	SER
1	A	132	LEU
1	A	165	LYS
1	A	199	THR
1	A	200	LYS
1	A	217	ILE
1	A	231	ASN
1	A	232	THR

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Mol	Chain	Res	Type
1	A	235	THR
1	A	237	ARG
1	A	242	THR
1	A	254	GLU
1	A	266	ILE
1	A	279	ASP
1	A	292	LEU
1	A	296	VAL
1	A	304	LEU
1	A	308	THR
1	A	316	LYS
1	A	319	LEU
1	A	338	LEU
1	A	344	LEU
1	A	362	ARG
1	A	368	LEU
1	A	389	GLN
1	A	390	ILE
1	A	404	ILE
1	A	408	GLU
1	A	416	VAL
1	A	425	VAL
1	A	466	ILE
1	A	470	VAL
1	A	477	CYS
1	A	479	GLN
1	A	512	GLU
1	A	513	GLU
1	A	531	LEU
1	A	549	LEU
1	A	569	ASP
1	A	578	ASP
1	A	605	VAL
1	A	612	LEU
1	A	615	VAL
1	A	619	LYS
1	A	626	SER
1	A	635	SER
1	A	636	LEU
1	A	640	ASP
1	A	658	LEU
1	A	670	ILE

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Mol	Chain	Res	Type
1	A	674	VAL
1	A	691	ILE
1	A	692	VAL
1	A	703	VAL
1	A	704	GLN
1	A	717	ARG
1	A	726	GLU
1	A	752	GLN
1	A	789	LYS
1	A	792	ILE
1	A	793	ASN
1	A	795	HIS
1	A	832	LEU
1	A	839	LEU
1	A	848	LEU
1	A	866	ILE
1	A	880	GLU
1	A	881	LEU
1	A	895	LYS
1	A	969	LEU
1	A	978	GLU
1	A	999	LYS
1	A	1027	GLN
1	A	1047	ILE
1	A	1057	ARG
1	A	1060	LYS
1	A	1086	THR
1	A	1093	ARG
1	A	1103	MET
1	A	1110	ILE
1	A	1117	THR
1	A	1130	ILE
1	A	1151	GLU
1	A	1154	ILE
1	A	1185	MET
1	A	1224	LEU
1	A	1230	HIS
1	A	1240	ILE
1	A	1247	SER
1	A	1252	THR
1	A	1312	GLU
1	B	8	ASP

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Mol	Chain	Res	Type
1	B	11	ILE
1	B	20	THR
1	B	28	VAL
1	B	36	LYS
1	B	43	THR
1	B	44	LYS
1	B	59	ILE
1	B	66	SER
1	B	97	SER
1	B	115	THR
1	B	127	SER
1	B	132	LEU
1	B	165	LYS
1	B	199	THR
1	B	216	LEU
1	B	217	ILE
1	B	231	ASN
1	B	232	THR
1	B	235	THR
1	B	237	ARG
1	B	242	THR
1	B	254	GLU
1	B	266	ILE
1	B	292	LEU
1	B	296	VAL
1	B	297	VAL
1	B	304	LEU
1	B	308	THR
1	B	316	LYS
1	B	338	LEU
1	B	344	LEU
1	B	362	ARG
1	B	368	LEU
1	B	389	GLN
1	B	390	ILE
1	B	397	LEU
1	B	404	ILE
1	B	408	GLU
1	B	415	PHE
1	B	416	VAL
1	B	425	VAL
1	B	466	ILE

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Mol	Chain	Res	Type
1	B	470	VAL
1	B	477	CYS
1	B	479	GLN
1	B	489	MET
1	B	502	SER
1	B	512	GLU
1	B	513	GLU
1	B	523	LEU
1	B	531	LEU
1	B	549	LEU
1	B	569	ASP
1	B	578	ASP
1	B	605	VAL
1	B	612	LEU
1	B	615	VAL
1	B	619	LYS
1	B	635	SER
1	B	636	LEU
1	B	640	ASP
1	B	658	LEU
1	B	670	ILE
1	B	674	VAL
1	B	691	ILE
1	B	692	VAL
1	B	703	VAL
1	B	704	GLN
1	B	717	ARG
1	B	720	GLU
1	B	728	PHE
1	B	752	GLN
1	B	789	LYS
1	B	792	ILE
1	B	793	ASN
1	B	795	HIS
1	B	832	LEU
1	B	839	LEU
1	B	848	LEU
1	B	866	ILE
1	B	880	GLU
1	B	881	LEU
1	B	938	LYS
1	B	969	LEU

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Mol	Chain	Res	Type
1	B	978	GLU
1	B	999	LYS
1	B	1027	GLN
1	B	1047	ILE
1	B	1057	ARG
1	B	1060	LYS
1	B	1086	THR
1	B	1093	ARG
1	B	1103	MET
1	B	1110	ILE
1	B	1117	THR
1	B	1130	ILE
1	B	1139	ARG
1	B	1151	GLU
1	B	1154	ILE
1	B	1185	MET
1	B	1224	LEU
1	B	1230	HIS
1	B	1240	ILE
1	B	1247	SER
1	B	1252	THR
1	B	1295	ILE
1	B	1312	GLU
1	B	1316	THR
1	C	8	ASP
1	C	11	ILE
1	C	20	THR
1	C	28	VAL
1	C	36	LYS
1	C	43	THR
1	C	44	LYS
1	C	59	ILE
1	C	66	SER
1	C	97	SER
1	C	115	THR
1	C	127	SER
1	C	132	LEU
1	C	165	LYS
1	C	199	THR
1	C	217	ILE
1	C	231	ASN
1	C	232	THR

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Mol	Chain	Res	Type
1	C	235	THR
1	C	237	ARG
1	C	242	THR
1	C	254	GLU
1	C	266	ILE
1	C	292	LEU
1	C	304	LEU
1	C	308	THR
1	C	316	LYS
1	C	319	LEU
1	C	338	LEU
1	C	344	LEU
1	C	362	ARG
1	C	368	LEU
1	C	390	ILE
1	C	404	ILE
1	C	415	PHE
1	C	416	VAL
1	C	425	VAL
1	C	466	ILE
1	C	470	VAL
1	C	477	CYS
1	C	479	GLN
1	C	505	MET
1	C	512	GLU
1	C	531	LEU
1	C	549	LEU
1	C	578	ASP
1	C	605	VAL
1	C	612	LEU
1	C	615	VAL
1	C	619	LYS
1	C	635	SER
1	C	636	LEU
1	C	640	ASP
1	C	658	LEU
1	C	670	ILE
1	C	674	VAL
1	C	691	ILE
1	C	692	VAL
1	C	703	VAL
1	C	704	GLN

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Mol	Chain	Res	Type
1	C	717	ARG
1	C	752	GLN
1	C	789	LYS
1	C	792	ILE
1	C	793	ASN
1	C	832	LEU
1	C	839	LEU
1	C	848	LEU
1	C	866	ILE
1	C	880	GLU
1	C	881	LEU
1	C	969	LEU
1	C	978	GLU
1	C	999	LYS
1	C	1027	GLN
1	C	1047	ILE
1	C	1057	ARG
1	C	1086	THR
1	C	1093	ARG
1	C	1103	MET
1	C	1110	ILE
1	C	1117	THR
1	C	1130	ILE
1	C	1139	ARG
1	C	1144	ASP
1	C	1151	GLU
1	C	1154	ILE
1	C	1185	MET
1	C	1224	LEU
1	C	1230	HIS
1	C	1240	ILE
1	C	1247	SER
1	C	1252	THR
1	C	1316	THR
1	C	1318	LEU
1	D	8	ASP
1	D	11	ILE
1	D	20	THR
1	D	28	VAL
1	D	36	LYS
1	D	43	THR
1	D	44	LYS

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Mol	Chain	Res	Type
1	D	59	ILE
1	D	66	SER
1	D	97	SER
1	D	115	THR
1	D	127	SER
1	D	132	LEU
1	D	165	LYS
1	D	199	THR
1	D	200	LYS
1	D	216	LEU
1	D	217	ILE
1	D	231	ASN
1	D	232	THR
1	D	235	THR
1	D	237	ARG
1	D	242	THR
1	D	266	ILE
1	D	279	ASP
1	D	292	LEU
1	D	299	ASN
1	D	304	LEU
1	D	308	THR
1	D	316	LYS
1	D	338	LEU
1	D	343	THR
1	D	344	LEU
1	D	362	ARG
1	D	368	LEU
1	D	376	ASN
1	D	389	GLN
1	D	390	ILE
1	D	404	ILE
1	D	408	GLU
1	D	415	PHE
1	D	416	VAL
1	D	425	VAL
1	D	466	ILE
1	D	470	VAL
1	D	512	GLU
1	D	523	LEU
1	D	531	LEU
1	D	549	LEU

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Mol	Chain	Res	Type
1	D	569	ASP
1	D	578	ASP
1	D	605	VAL
1	D	612	LEU
1	D	615	VAL
1	D	619	LYS
1	D	626	SER
1	D	635	SER
1	D	636	LEU
1	D	640	ASP
1	D	658	LEU
1	D	670	ILE
1	D	674	VAL
1	D	691	ILE
1	D	692	VAL
1	D	703	VAL
1	D	717	ARG
1	D	752	GLN
1	D	789	LYS
1	D	792	ILE
1	D	832	LEU
1	D	839	LEU
1	D	848	LEU
1	D	866	ILE
1	D	881	LEU
1	D	969	LEU
1	D	978	GLU
1	D	1027	GLN
1	D	1047	ILE
1	D	1057	ARG
1	D	1060	LYS
1	D	1086	THR
1	D	1093	ARG
1	D	1103	MET
1	D	1110	ILE
1	D	1117	THR
1	D	1130	ILE
1	D	1154	ILE
1	D	1185	MET
1	D	1224	LEU
1	D	1230	HIS
1	D	1240	ILE

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Mol	Chain	Res	Type
1	D	1247	SER
1	D	1252	THR
1	D	1288	GLU
1	D	1312	GLU
1	D	1316	THR

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

Mol	Chain	Res	Type
1	A	208	GLN
1	A	268	ASN
1	A	317	ASN
1	A	388	GLN
1	A	574	GLN
1	A	704	GLN
1	A	721	GLN
1	A	733	GLN
1	A	857	ASN
1	A	871	ASN
1	A	971	GLN
1	A	1048	ASN
1	A	1067	HIS
1	A	1091	ASN
1	A	1097	ASN
1	A	1100	GLN
1	A	1254	ASN
1	B	208	GLN
1	B	268	ASN
1	B	317	ASN
1	B	388	GLN
1	B	704	GLN
1	B	733	GLN
1	B	752	GLN
1	B	971	GLN
1	B	984	ASN
1	B	1067	HIS
1	B	1091	ASN
1	B	1097	ASN
1	B	1100	GLN
1	B	1254	ASN
1	C	268	ASN
1	C	317	ASN

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Mol	Chain	Res	Type
1	C	376	ASN
1	C	380	ASN
1	C	587	GLN
1	C	704	GLN
1	C	721	GLN
1	C	752	GLN
1	C	772	GLN
1	C	857	ASN
1	C	867	GLN
1	C	871	ASN
1	C	1048	ASN
1	C	1067	HIS
1	C	1091	ASN
1	C	1097	ASN
1	C	1100	GLN
1	C	1254	ASN
1	D	150	ASN
1	D	208	GLN
1	D	317	ASN
1	D	551	HIS
1	D	708	GLN
1	D	721	GLN
1	D	752	GLN
1	D	857	ASN
1	D	871	ASN
1	D	971	GLN
1	D	1091	ASN
1	D	1097	ASN
1	D	1100	GLN
1	D	1254	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 for Mogul analysis.

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
6	FAD	C	3005	-	58,58,58	1.46	10 (17%)	85,89,89	1.54	16 (18%)
6	FAD	D	3005	-	58,58,58	1.44	8 (13%)	85,89,89	1.56	15 (17%)
6	FAD	A	3005	-	58,58,58	1.44	9 (15%)	85,89,89	1.56	16 (18%)
6	FAD	B	3005	-	58,58,58	1.45	9 (15%)	85,89,89	1.69	21 (24%)
5	MOS	A	3004	4	0,3,3	-	-	-		
5	MOS	B	3004	4	0,3,3	-	-	-		
5	MOS	C	3004	4	0,3,3	-	-	-		
3	FES	B	3002	1	0,4,4	-	-	-		
3	FES	A	3001	1	0,4,4	-	-	-		
4	MTE	D	3003	5	21,26,26	1.55	2 (9%)	19,40,40	1.93	5 (26%)
3	FES	B	3001	1	0,4,4	-	-	-		
5	MOS	D	3004	4	0,3,3	-	-	-		
3	FES	C	3001	1	0,4,4	-	-	-		
3	FES	A	3002	1	0,4,4	-	-	-		
3	FES	D	3002	1	0,4,4	-	-	-		
3	FES	D	3001	1	0,4,4	-	-	-		
3	FES	C	3002	1	0,4,4	-	-	-		
4	MTE	C	3003	5	21,26,26	1.55	3 (14%)	19,40,40	2.43	6 (31%)
4	MTE	B	3003	5	21,26,26	1.53	2 (9%)	19,40,40	2.25	7 (36%)
4	MTE	A	3003	5	21,26,26	1.50	2 (9%)	19,40,40	2.06	6 (31%)

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
3	FES	D	3001	1	-	-	0/1/1/1
4	MTE	D	3003	5	-	4/6/34/34	0/3/3/3
6	FAD	C	3005	-	-	17/34/50/50	0/6/6/6
6	FAD	D	3005	-	-	12/34/50/50	0/6/6/6
6	FAD	A	3005	-	-	8/34/50/50	0/6/6/6
6	FAD	B	3005	-	-	17/34/50/50	0/6/6/6
3	FES	B	3002	1	-	-	0/1/1/1
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	C	3002	1	-	-	0/1/1/1
4	MTE	C	3003	5	-	0/6/34/34	0/3/3/3
3	FES	C	3001	1	-	-	0/1/1/1
3	FES	A	3002	1	-	-	0/1/1/1
4	MTE	B	3003	5	-	2/6/34/34	0/3/3/3
3	FES	B	3001	1	-	-	0/1/1/1
3	FES	D	3002	1	-	-	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3003	MTE	C9-C10	5.63	1.48	1.38
6	B	3005	FAD	C9A-C5X	5.35	1.49	1.41
6	C	3005	FAD	C9A-C5X	5.30	1.49	1.41
4	C	3003	MTE	C9-C10	5.28	1.47	1.38
4	A	3003	MTE	C9-C10	5.24	1.47	1.38
4	D	3003	MTE	C9-C10	5.18	1.47	1.38
6	D	3005	FAD	C9A-C5X	5.08	1.49	1.41
6	A	3005	FAD	C9A-C5X	5.07	1.49	1.41
6	A	3005	FAD	C5A-C4A	4.45	1.47	1.39
6	C	3005	FAD	C5A-C4A	4.44	1.47	1.39
6	B	3005	FAD	C5A-C4A	4.34	1.46	1.39
6	D	3005	FAD	C5A-C4A	4.30	1.46	1.39
6	B	3005	FAD	C8-C7	3.38	1.49	1.40
6	D	3005	FAD	C8-C7	3.33	1.49	1.40
6	C	3005	FAD	C8-C7	3.28	1.48	1.40
6	A	3005	FAD	C8-C7	3.20	1.48	1.40
6	D	3005	FAD	C4-N3	-2.89	1.33	1.38
6	A	3005	FAD	C4-N3	-2.74	1.33	1.38
6	B	3005	FAD	C4-N3	-2.74	1.33	1.38
6	C	3005	FAD	C5A-C6A	2.68	1.48	1.41
6	A	3005	FAD	C5A-C6A	2.66	1.48	1.41
4	D	3003	MTE	C4-N3	-2.63	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3005	FAD	C4-N3	-2.63	1.33	1.38
6	D	3005	FAD	C5A-N7A	-2.61	1.34	1.39
6	D	3005	FAD	C5A-C6A	2.57	1.48	1.41
6	A	3005	FAD	C5A-N7A	-2.56	1.34	1.39
6	B	3005	FAD	C5A-C6A	2.51	1.48	1.41
6	B	3005	FAD	C5A-N7A	-2.48	1.34	1.39
6	D	3005	FAD	C5X-N5	-2.44	1.34	1.39
4	C	3003	MTE	C4-N3	-2.43	1.34	1.38
6	C	3005	FAD	C5X-N5	-2.39	1.35	1.39
6	A	3005	FAD	C5X-N5	-2.37	1.35	1.39
6	B	3005	FAD	C5X-N5	-2.36	1.35	1.39
6	C	3005	FAD	C5A-N7A	-2.36	1.34	1.39
4	A	3003	MTE	C4-N3	-2.32	1.34	1.38
6	C	3005	FAD	C8A-N7A	2.26	1.36	1.31
4	B	3003	MTE	C4-N3	-2.20	1.34	1.38
6	C	3005	FAD	C4A-N9A	-2.12	1.33	1.37
6	A	3005	FAD	C8A-N7A	2.11	1.35	1.31
6	B	3005	FAD	C4A-N9A	-2.10	1.33	1.37
6	A	3005	FAD	C2-N3	-2.08	1.34	1.39
6	B	3005	FAD	C2-N3	-2.05	1.34	1.39
6	C	3005	FAD	C2-N3	-2.03	1.34	1.39
6	D	3005	FAD	C8A-N7A	2.03	1.35	1.31
4	C	3003	MTE	C9-C4	2.00	1.47	1.41

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3003	MTE	O3'-C7-C6	-7.24	104.14	108.96
6	A	3005	FAD	C5A-C4A-N3A	-5.98	118.48	126.72
6	D	3005	FAD	C5A-C4A-N3A	-5.95	118.53	126.72
6	C	3005	FAD	C5A-C4A-N3A	-5.54	119.08	126.72
6	B	3005	FAD	C5A-C4A-N3A	-5.51	119.13	126.72
6	A	3005	FAD	N3A-C4A-N9A	4.73	135.22	127.17
6	D	3005	FAD	N3A-C4A-N9A	4.71	135.18	127.17
6	B	3005	FAD	C1'-N10-C9A	4.67	129.70	120.63
6	B	3005	FAD	N3A-C4A-N9A	4.55	134.91	127.17
4	D	3003	MTE	C2-N1-C10	4.47	121.24	113.36
4	B	3003	MTE	C2-N1-C10	4.45	121.22	113.36
4	B	3003	MTE	O3'-C7-C6	-4.32	106.08	108.96
6	C	3005	FAD	N3A-C4A-N9A	4.32	134.52	127.17
4	C	3003	MTE	C2-N1-C10	4.22	120.80	113.36
4	A	3003	MTE	O3'-C7-N8	4.20	112.42	108.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3003	MTE	C2-N1-C10	4.19	120.75	113.36
6	D	3005	FAD	C2A-N3A-C4A	3.75	121.00	111.83
6	A	3005	FAD	C2A-N3A-C4A	3.72	120.92	111.83
6	B	3005	FAD	C2A-N3A-C4A	3.67	120.79	111.83
4	D	3003	MTE	O3'-C7-C6	-3.66	106.52	108.96
6	C	3005	FAD	C2A-N3A-C4A	3.61	120.66	111.83
6	A	3005	FAD	C4A-C5A-N7A	-3.61	106.46	110.58
6	C	3005	FAD	C4A-C5A-N7A	-3.60	106.47	110.58
4	B	3003	MTE	O4-C4-C9	-3.55	118.70	127.26
6	B	3005	FAD	N3A-C2A-N1A	-3.52	123.25	128.58
6	D	3005	FAD	C4A-C5A-N7A	-3.41	106.68	110.58
4	A	3003	MTE	O4-C4-C9	-3.39	119.08	127.26
6	D	3005	FAD	N3A-C2A-N1A	-3.30	123.59	128.58
6	B	3005	FAD	C4X-C10-N10	3.25	121.14	116.48
6	B	3005	FAD	C4A-C5A-N7A	-3.25	106.87	110.58
6	C	3005	FAD	N3A-C2A-N1A	-3.19	123.76	128.58
6	A	3005	FAD	N3A-C2A-N1A	-3.09	123.91	128.58
6	B	3005	FAD	C2'-C1'-N10	3.03	124.52	110.20
4	D	3003	MTE	O4-C4-C9	-3.00	120.02	127.26
6	B	3005	FAD	C4-C4X-N5	2.96	122.29	118.21
6	B	3005	FAD	C4A-N9A-C8A	2.92	108.80	105.74
6	C	3005	FAD	C4A-N9A-C8A	2.88	108.77	105.74
4	C	3003	MTE	O4-C4-C9	-2.84	120.42	127.26
4	A	3003	MTE	O3'-C7-C6	-2.77	107.12	108.96
4	B	3003	MTE	O3'-C7-N8	2.76	111.11	108.61
6	A	3005	FAD	C4A-N9A-C8A	2.69	108.56	105.74
6	A	3005	FAD	C5A-N7A-C8A	2.68	107.66	103.45
6	C	3005	FAD	C4-C4X-N5	2.66	121.89	118.21
6	C	3005	FAD	C5A-N7A-C8A	2.66	107.62	103.45
6	D	3005	FAD	C4X-C10-N1	-2.63	118.14	124.59
6	A	3005	FAD	C4X-C10-N1	-2.61	118.18	124.59
6	D	3005	FAD	C5A-N7A-C8A	2.61	107.55	103.45
4	D	3003	MTE	C9-C4-N3	2.52	119.06	112.13
6	C	3005	FAD	C4X-C10-N10	2.51	120.07	116.48
6	A	3005	FAD	C4-C4X-N5	2.51	121.67	118.21
6	D	3005	FAD	C4-C4X-N5	2.50	121.67	118.21
6	D	3005	FAD	C4A-N9A-C8A	2.50	108.36	105.74
4	B	3003	MTE	C9-C4-N3	2.48	118.94	112.13
6	B	3005	FAD	C5A-N7A-C8A	2.46	107.32	103.45
6	A	3005	FAD	C4X-C10-N10	2.42	119.95	116.48
6	C	3005	FAD	O4-C4-C4X	-2.41	120.17	126.53
4	A	3003	MTE	C9-C4-N3	2.40	118.72	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3005	FAD	C4X-C10-N1	-2.40	118.71	124.59
6	B	3005	FAD	C4X-C10-N1	-2.35	118.83	124.59
4	C	3003	MTE	C4-C9-N5	2.35	122.67	116.27
6	B	3005	FAD	O4-C4-C4X	-2.31	120.42	126.53
6	C	3005	FAD	C6A-C5A-N7A	2.31	136.55	132.09
4	A	3003	MTE	C4-C9-N5	2.31	122.57	116.27
4	C	3003	MTE	O2P-P-O4'	-2.29	100.71	106.67
6	B	3005	FAD	C9A-N10-C10	-2.28	117.28	120.75
4	D	3003	MTE	C4-C9-N5	2.26	122.43	116.27
4	C	3003	MTE	C9-C4-N3	2.26	118.33	112.13
6	D	3005	FAD	O4-C4-C4X	-2.25	120.58	126.53
6	C	3005	FAD	N9A-C8A-N7A	-2.25	110.74	113.94
6	D	3005	FAD	C4X-C10-N10	2.23	119.67	116.48
6	A	3005	FAD	O4-C4-C4X	-2.22	120.68	126.53
6	B	3005	FAD	O2-C2-N1	-2.19	118.16	121.80
4	B	3003	MTE	C2-N3-C4	-2.17	121.17	125.11
6	B	3005	FAD	C6A-C5A-N7A	2.16	136.25	132.09
6	A	3005	FAD	C10-N1-C2	2.11	121.42	116.85
6	C	3005	FAD	O2-C2-N1	-2.11	118.30	121.80
4	B	3003	MTE	O3P-P-O2P	2.09	115.65	107.80
6	B	3005	FAD	C2A-N1A-C6A	2.08	122.15	118.73
6	B	3005	FAD	C5'-C4'-C3'	-2.07	108.32	112.22
6	A	3005	FAD	C6A-C5A-N7A	2.07	136.07	132.09
6	A	3005	FAD	C4-N3-C2	-2.07	121.97	125.64
6	D	3005	FAD	C10-N1-C2	2.06	121.32	116.85
6	A	3005	FAD	N9A-C8A-N7A	-2.06	111.02	113.94
6	D	3005	FAD	C4-N3-C2	-2.06	121.99	125.64
6	D	3005	FAD	C4X-C4-N3	2.04	118.45	113.25
6	B	3005	FAD	C10-N1-C2	2.04	121.26	116.85
6	B	3005	FAD	N9A-C8A-N7A	-2.04	111.05	113.94
6	C	3005	FAD	C10-N1-C2	2.03	121.25	116.85
6	B	3005	FAD	C4X-C4-N3	2.03	118.43	113.25
6	C	3005	FAD	C4X-C4-N3	2.02	118.40	113.25
6	A	3005	FAD	C4X-C4-N3	2.01	118.37	113.25
6	D	3005	FAD	C6A-C5A-N7A	2.01	135.96	132.09

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	3003	MTE	C4'-O4'-P-O1P
4	D	3003	MTE	C4'-O4'-P-O2P

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Mol	Chain	Res	Type	Atoms
4	D	3003	MTE	C4'-O4'-P-O3P
6	A	3005	FAD	C5B-O5B-PA-O2A
6	B	3005	FAD	C5B-O5B-PA-O1A
6	B	3005	FAD	C5B-O5B-PA-O2A
6	B	3005	FAD	C5B-O5B-PA-O3P
6	B	3005	FAD	C2'-C1'-N10-C9A
6	B	3005	FAD	C2'-C1'-N10-C10
6	B	3005	FAD	N10-C1'-C2'-O2'
6	B	3005	FAD	N10-C1'-C2'-C3'
6	B	3005	FAD	C1'-C2'-C3'-C4'
6	B	3005	FAD	C5'-O5'-P-O1P
6	B	3005	FAD	C5'-O5'-P-O2P
6	B	3005	FAD	C5'-O5'-P-O3P
6	C	3005	FAD	C5B-O5B-PA-O1A
6	C	3005	FAD	C2'-C1'-N10-C9A
6	C	3005	FAD	C2'-C1'-N10-C10
6	C	3005	FAD	N10-C1'-C2'-O2'
6	C	3005	FAD	N10-C1'-C2'-C3'
6	C	3005	FAD	C1'-C2'-C3'-O3'
6	C	3005	FAD	C1'-C2'-C3'-C4'
6	C	3005	FAD	O2'-C2'-C3'-O3'
6	C	3005	FAD	O2'-C2'-C3'-C4'
6	D	3005	FAD	C5B-O5B-PA-O1A
6	D	3005	FAD	C5B-O5B-PA-O2A
6	D	3005	FAD	C5B-O5B-PA-O3P
6	D	3005	FAD	O4B-C4B-C5B-O5B
6	D	3005	FAD	C1'-C2'-C3'-O3'
6	D	3005	FAD	C1'-C2'-C3'-C4'
6	D	3005	FAD	O2'-C2'-C3'-O3'
6	D	3005	FAD	O2'-C2'-C3'-C4'
6	D	3005	FAD	C3'-C4'-C5'-O5'
6	D	3005	FAD	O4'-C4'-C5'-O5'
6	A	3005	FAD	C3B-C4B-C5B-O5B
6	B	3005	FAD	O4B-C4B-C5B-O5B
6	B	3005	FAD	C3B-C4B-C5B-O5B
6	A	3005	FAD	O4B-C4B-C5B-O5B
6	C	3005	FAD	O4B-C4B-C5B-O5B
6	C	3005	FAD	C3B-C4B-C5B-O5B
6	D	3005	FAD	C3B-C4B-C5B-O5B
4	D	3003	MTE	C3'-C4'-O4'-P
6	A	3005	FAD	C3'-C4'-C5'-O5'
4	B	3003	MTE	C4'-O4'-P-O1P

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Mol	Chain	Res	Type	Atoms
6	A	3005	FAD	O4'-C4'-C5'-O5'
6	B	3005	FAD	O2'-C2'-C3'-C4'
6	A	3005	FAD	C1'-C2'-C3'-O3'
6	B	3005	FAD	C1'-C2'-C3'-O3'
6	C	3005	FAD	C2'-C3'-C4'-O4'
6	B	3005	FAD	O2'-C2'-C3'-O3'
6	C	3005	FAD	O3'-C3'-C4'-O4'
6	A	3005	FAD	C5B-O5B-PA-O1A
6	A	3005	FAD	C5B-O5B-PA-O3P
6	C	3005	FAD	C5B-O5B-PA-O2A
6	C	3005	FAD	C5B-O5B-PA-O3P
6	C	3005	FAD	O3'-C3'-C4'-C5'
6	C	3005	FAD	C2'-C3'-C4'-C5'
4	B	3003	MTE	C4'-O4'-P-O3P
6	D	3005	FAD	N10-C1'-C2'-O2'
6	B	3005	FAD	PA-O3P-P-O2P

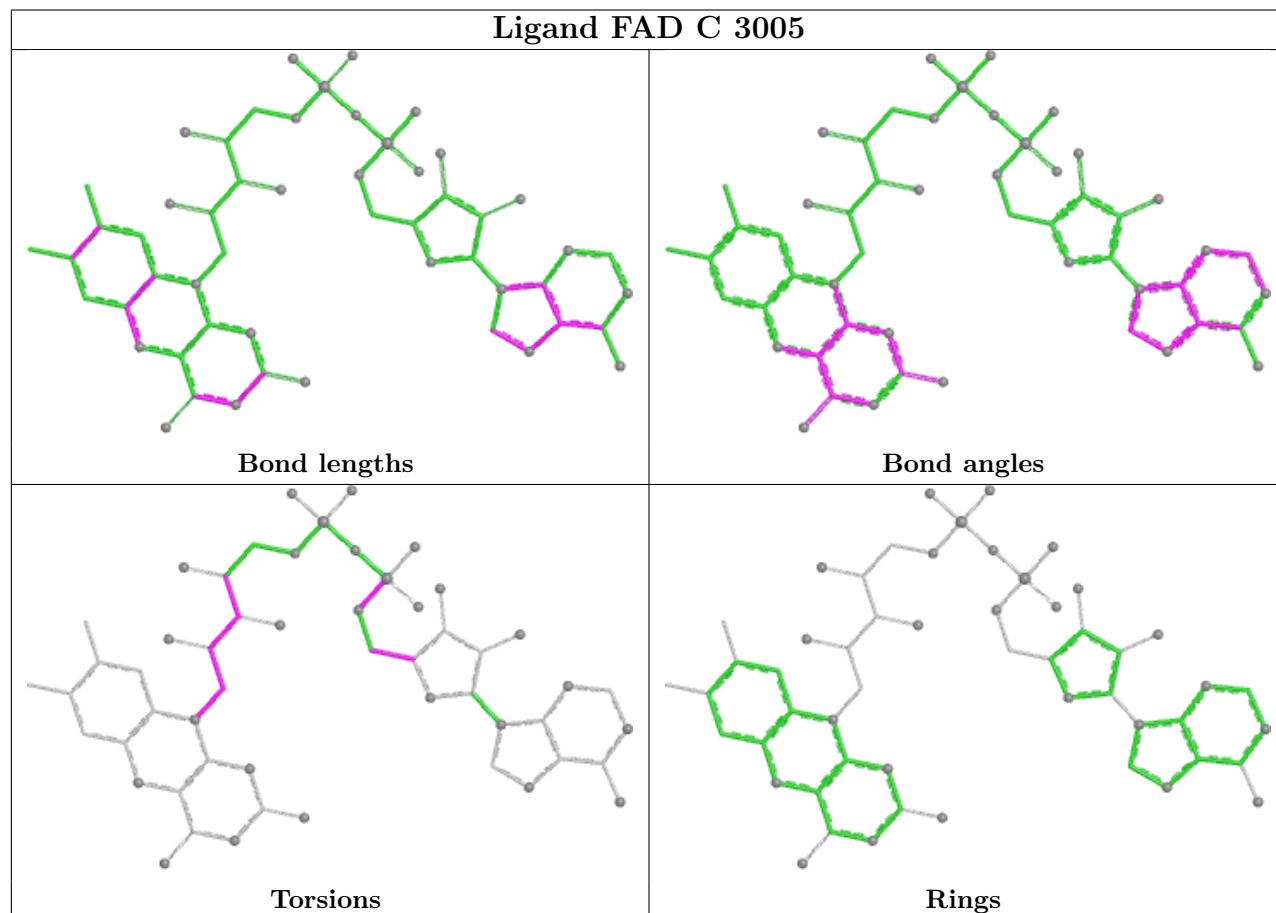
There are no ring outliers.

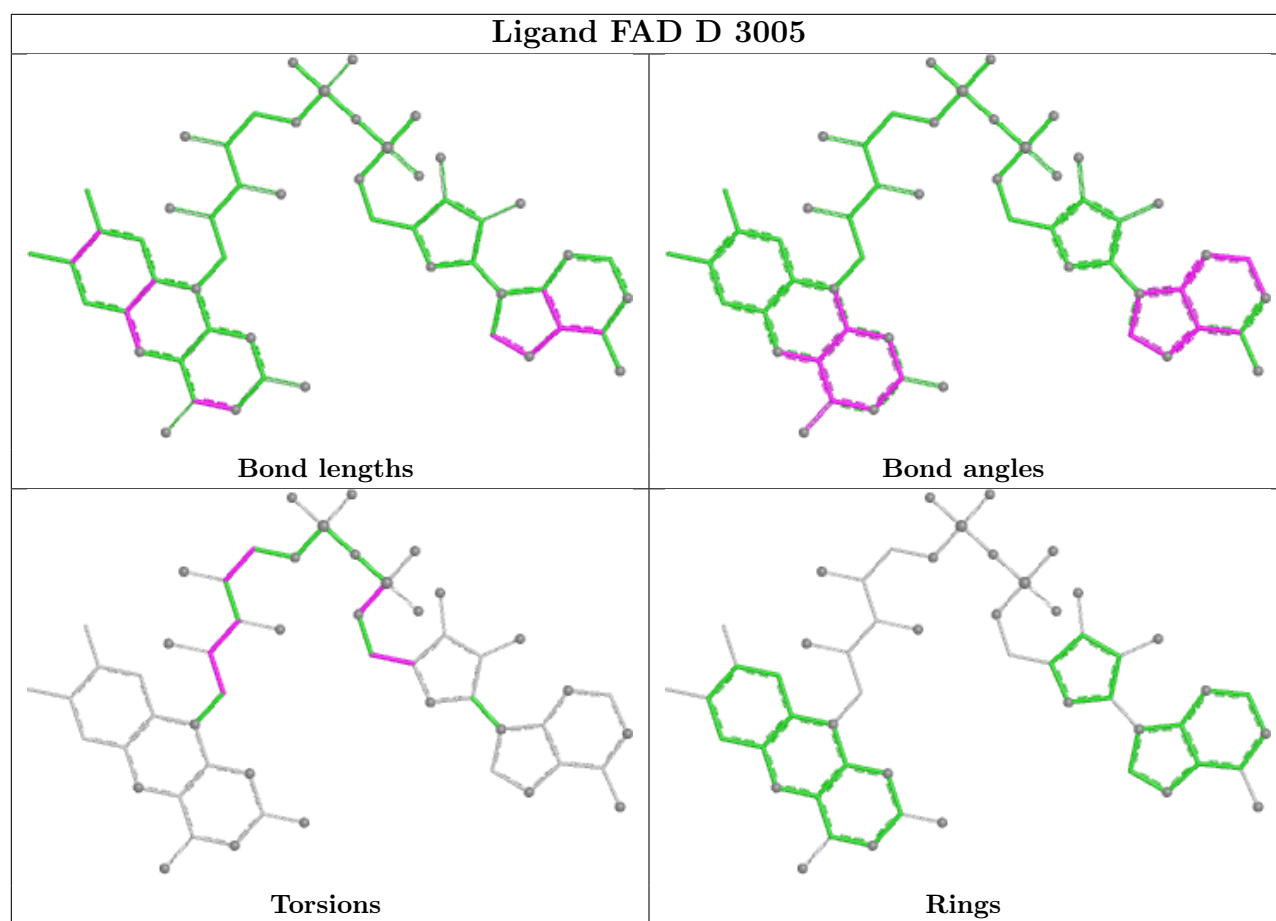
16 monomers are involved in 81 short contacts:

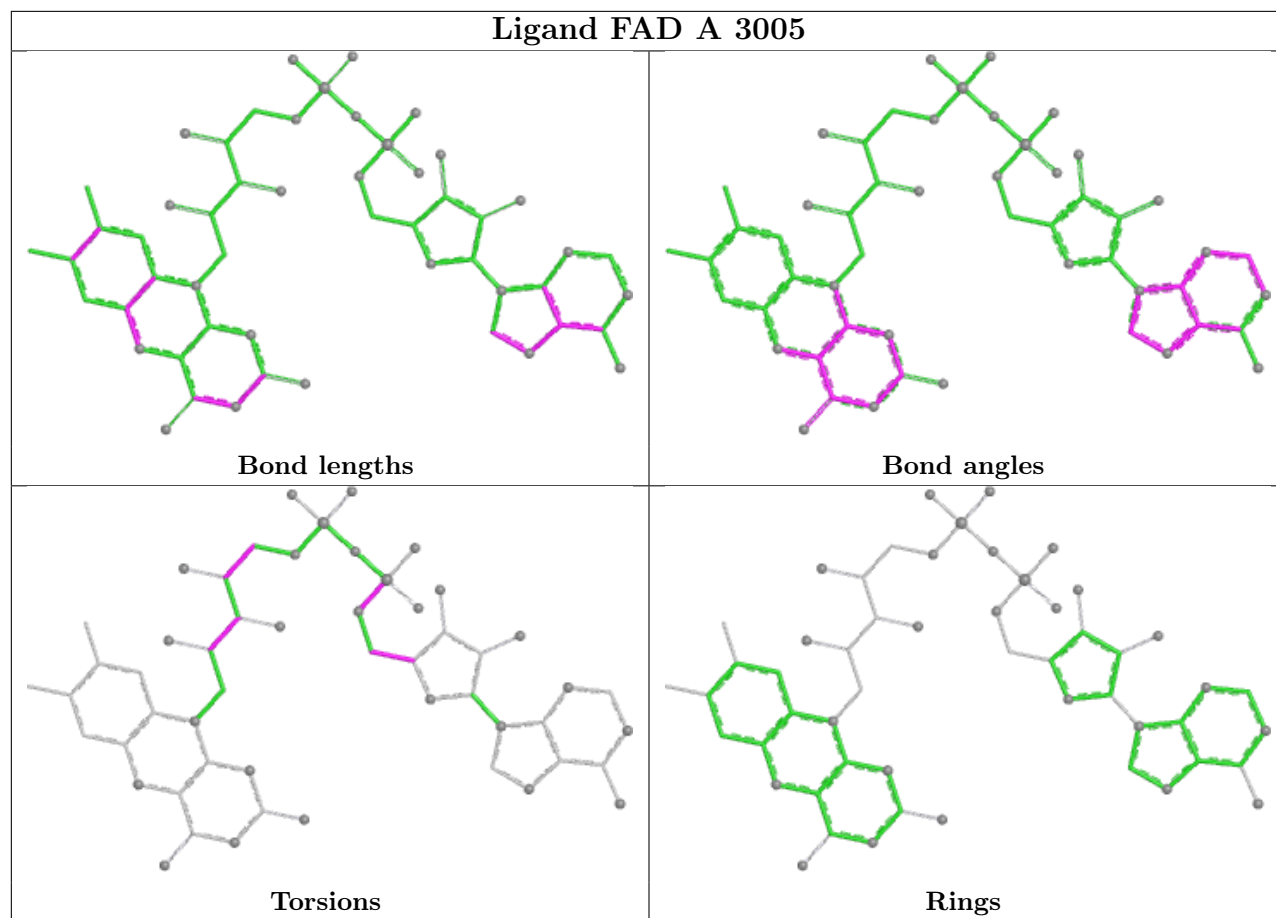
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3005	FAD	20	0
6	D	3005	FAD	15	0
6	A	3005	FAD	8	0
6	B	3005	FAD	14	0
5	A	3004	MOS	2	0
5	B	3004	MOS	2	0
5	C	3004	MOS	2	0
3	B	3002	FES	1	0
4	D	3003	MTE	3	0
5	D	3004	MOS	2	0
3	A	3002	FES	1	0
3	D	3002	FES	2	0
3	C	3002	FES	1	0
4	C	3003	MTE	3	0
4	B	3003	MTE	1	0
4	A	3003	MTE	4	0

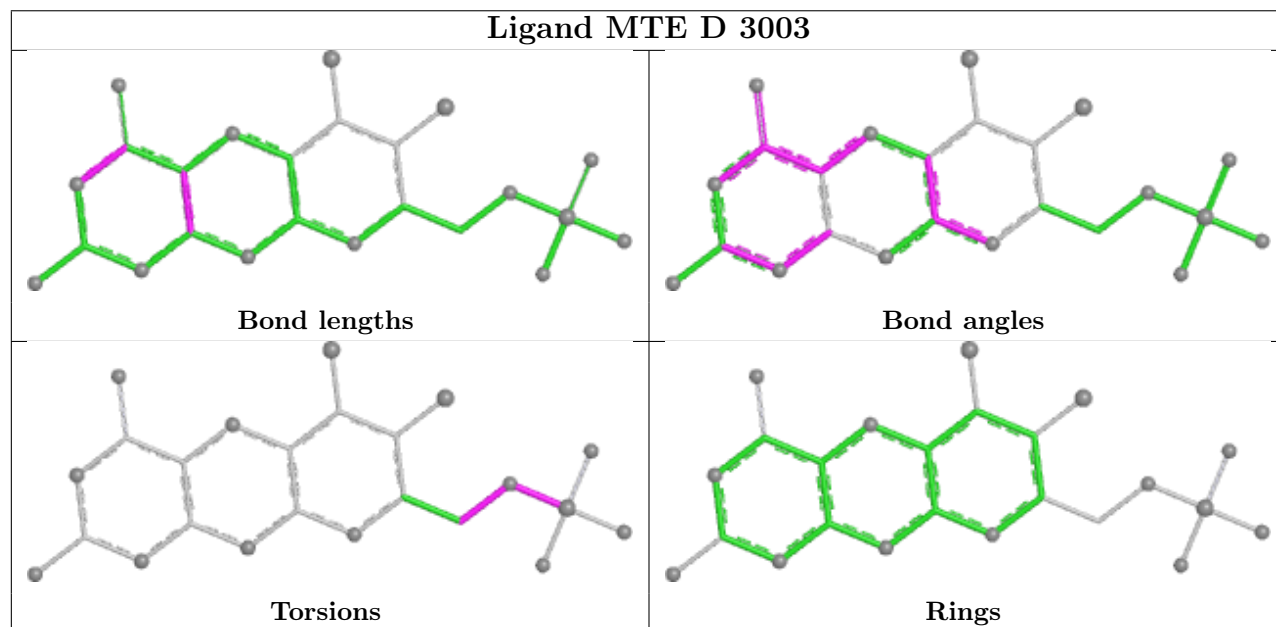
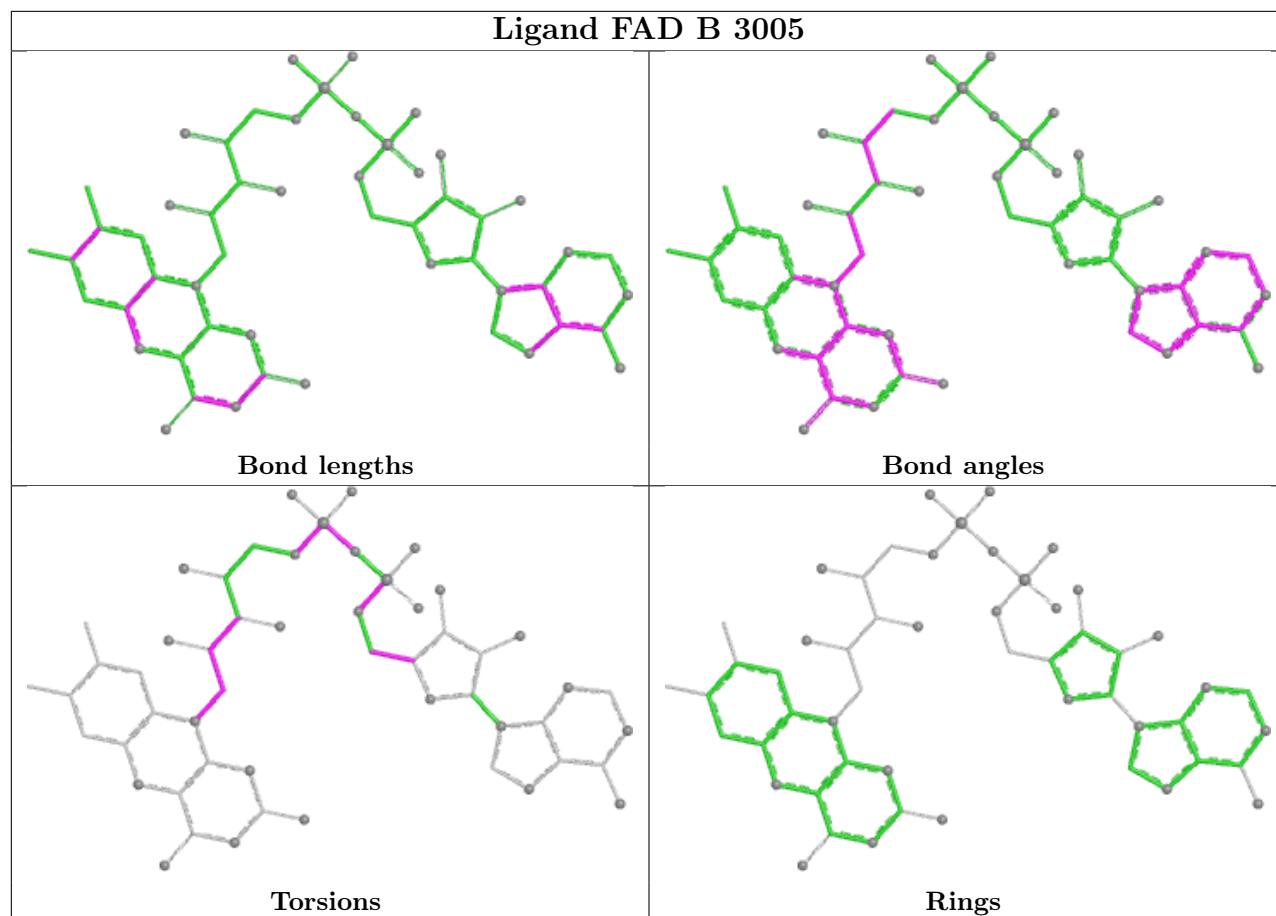
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

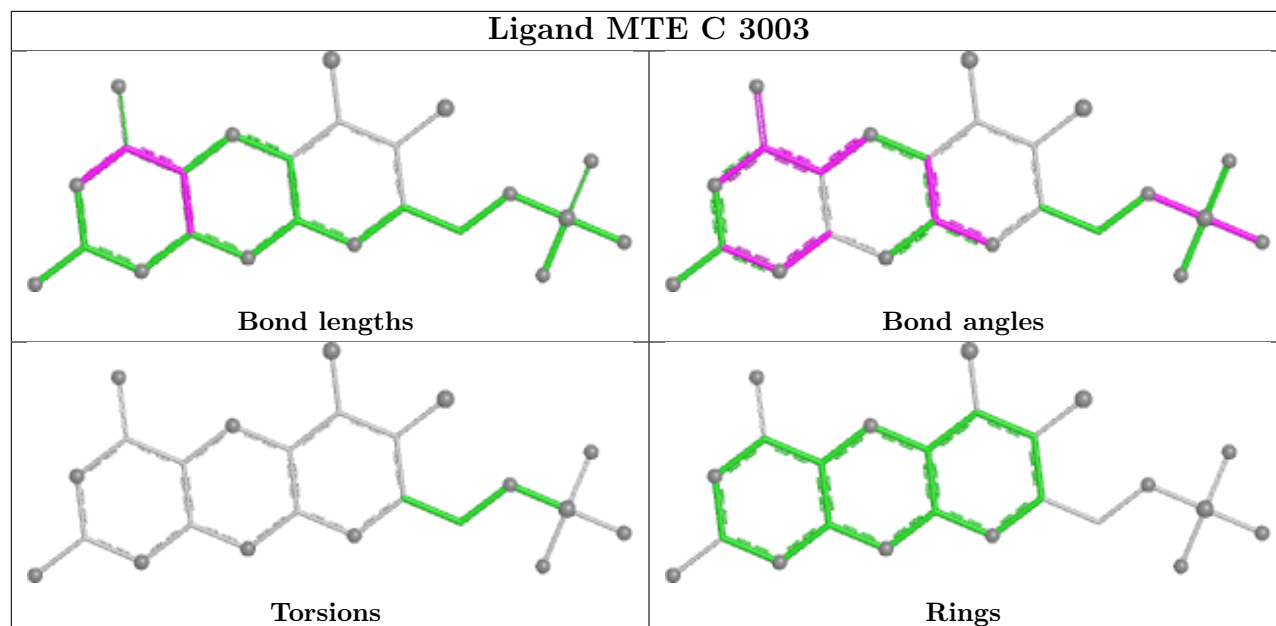




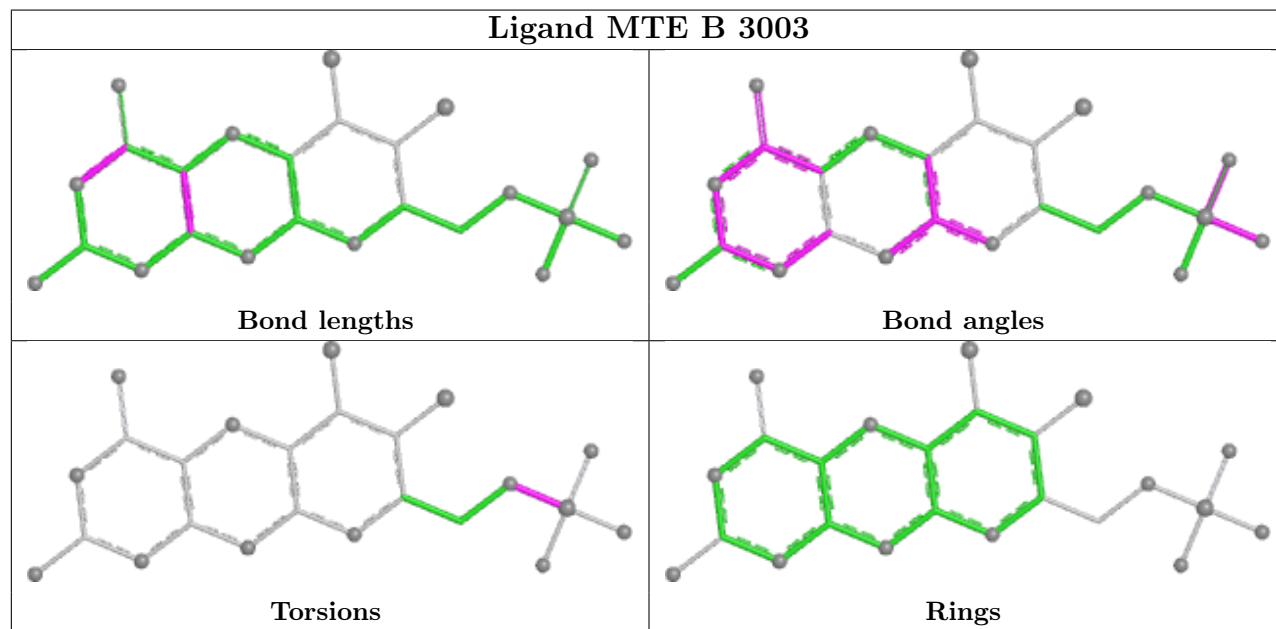


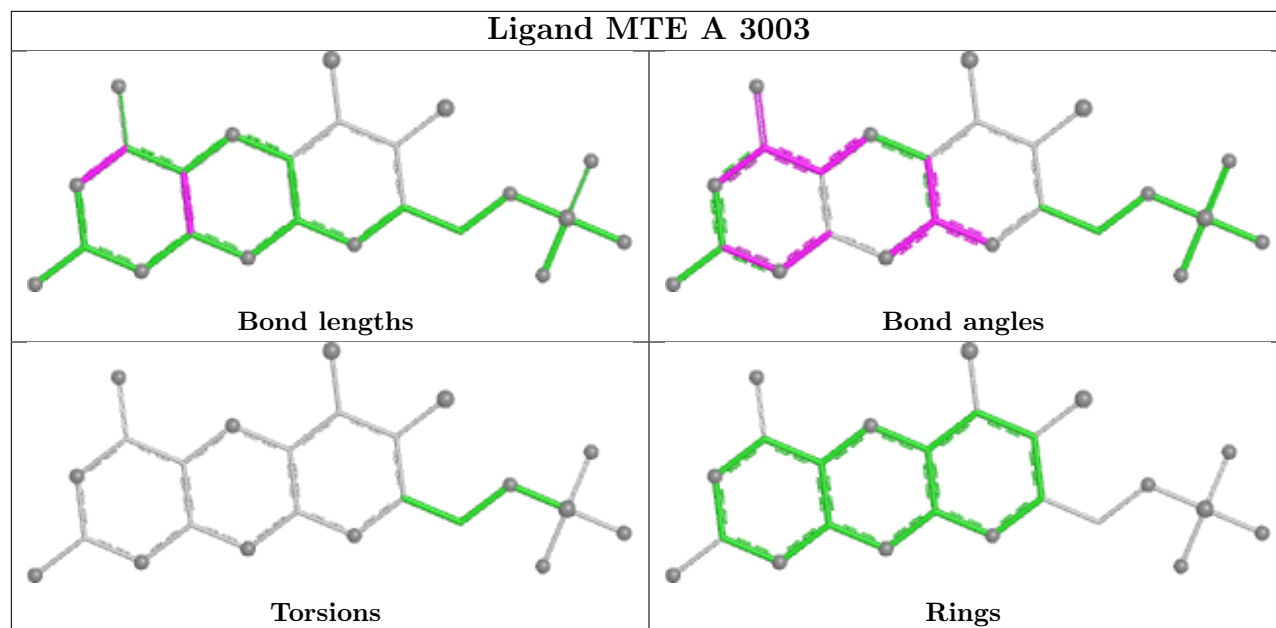


Ligand MTE C 3003



Ligand MTE B 3003





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	1253/1335 (93%)	0.62	95 (7%)	20	19	12, 40, 70, 88	0
1	B	1262/1335 (94%)	0.63	95 (7%)	20	19	10, 39, 67, 87	0
1	C	1244/1335 (93%)	0.72	95 (7%)	20	19	18, 43, 73, 99	0
1	D	1257/1335 (94%)	0.84	122 (9%)	13	12	20, 45, 79, 97	0
All	All	5016/5340 (93%)	0.70	407 (8%)	18	17	10, 42, 73, 99	0

All (407) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	CYS	5.5
1	D	278	THR	5.4
1	B	403	ALA	4.8
1	D	398	ALA	4.5
1	B	857	ASN	4.5
1	B	398	ALA	4.4
1	B	1228	GLY	4.2
1	C	491	ASP	4.2
1	D	545	ILE	4.1
1	C	424	PHE	4.1
1	D	335	CYS	4.1
1	D	274	HIS	4.1
1	D	548	LYS	4.0
1	D	377	CYS	4.0
1	B	727	ALA	3.9
1	D	899	LEU	3.9
1	A	447	VAL	3.9
1	D	538	ASP	3.8
1	B	728	PHE	3.7
1	B	1300	SER	3.7
1	A	424	PHE	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	277	PHE	3.7
1	A	376	ASN	3.7
1	C	869	TYR	3.7
1	B	323	VAL	3.6
1	C	734	ILE	3.6
1	A	489	MET	3.6
1	D	492	ASP	3.6
1	B	1252	THR	3.6
1	B	7	SER	3.6
1	C	7	SER	3.6
1	A	216	LEU	3.6
1	B	549	LEU	3.6
1	A	552	ILE	3.6
1	C	458	ASP	3.6
1	D	484	CYS	3.5
1	A	422	TRP	3.5
1	C	506	ALA	3.5
1	C	859	GLY	3.5
1	A	169	PRO	3.5
1	D	934	ALA	3.5
1	D	893	ALA	3.5
1	D	422	TRP	3.5
1	B	296	VAL	3.5
1	B	559	THR	3.5
1	C	988	ALA	3.4
1	D	1296	TRP	3.4
1	C	557	PRO	3.4
1	A	484	CYS	3.4
1	D	1295	ILE	3.4
1	B	1153	ASP	3.4
1	A	729	GLN	3.4
1	D	323	VAL	3.4
1	A	734	ILE	3.4
1	C	473	ALA	3.4
1	C	484	CYS	3.4
1	D	482	GLY	3.4
1	A	471	ILE	3.3
1	D	485	TRP	3.3
1	A	559	THR	3.3
1	A	481	ILE	3.3
1	B	896	ILE	3.3
1	C	937	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	1249	LEU	3.3
1	C	550	LEU	3.3
1	B	1107	GLU	3.3
1	C	447	VAL	3.3
1	D	927	VAL	3.3
1	D	1246	VAL	3.3
1	B	859	GLY	3.3
1	C	275	MET	3.3
1	C	711	SER	3.2
1	D	1228	GLY	3.2
1	A	1296	TRP	3.2
1	A	969	LEU	3.2
1	C	862	LYS	3.2
1	D	873	GLY	3.2
1	C	861	ILE	3.2
1	D	530	VAL	3.2
1	D	1083	GLY	3.2
1	B	863	ALA	3.2
1	D	459	LEU	3.2
1	A	466	ILE	3.2
1	D	549	LEU	3.1
1	B	377	CYS	3.1
1	A	485	TRP	3.1
1	D	734	ILE	3.1
1	B	557	PRO	3.1
1	C	942	PRO	3.1
1	A	420	SER	3.1
1	B	558	LEU	3.1
1	B	376	ASN	3.1
1	B	421	LYS	3.1
1	C	898	ASN	3.1
1	D	524	PHE	3.0
1	A	536	THR	3.0
1	D	1311	CYS	3.0
1	C	933	SER	3.0
1	A	852	LYS	3.0
1	D	961	ASN	3.0
1	B	425	VAL	3.0
1	C	848	LEU	3.0
1	C	524	PHE	3.0
1	A	417	PRO	3.0
1	B	531	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	1153	ASP	3.0
1	D	728	PHE	3.0
1	A	1150	GLY	3.0
1	D	1294	PRO	2.9
1	B	373	GLY	2.9
1	D	226	ALA	2.9
1	A	997	PHE	2.9
1	D	521	SER	2.9
1	C	466	ILE	2.9
1	D	461	ILE	2.9
1	D	896	ILE	2.9
1	C	698	PRO	2.9
1	D	1300	SER	2.8
1	C	274	HIS	2.8
1	B	338	LEU	2.8
1	C	854	GLY	2.8
1	B	1230	HIS	2.8
1	C	536	THR	2.8
1	B	1295	ILE	2.8
1	D	857	ASN	2.8
1	D	322	VAL	2.8
1	C	398	ALA	2.8
1	C	1285	ALA	2.8
1	D	1098	ALA	2.8
1	C	547	GLN	2.8
1	A	303	GLY	2.8
1	B	281	SER	2.8
1	D	858	ASN	2.8
1	A	280	VAL	2.8
1	C	949	LEU	2.8
1	C	1318	LEU	2.8
1	D	733	GLN	2.8
1	A	1146	ASP	2.8
1	C	303	GLY	2.7
1	B	861	ILE	2.7
1	B	952	TYR	2.7
1	B	576	LEU	2.7
1	A	1297	ALA	2.7
1	C	373	GLY	2.7
1	D	1306	VAL	2.7
1	A	490	LEU	2.7
1	A	468	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	729	GLN	2.7
1	A	458	ASP	2.7
1	D	297	VAL	2.7
1	A	576	LEU	2.7
1	C	1296	TRP	2.7
1	B	507	ALA	2.7
1	C	954	THR	2.7
1	B	492	ASP	2.7
1	A	477	CYS	2.7
1	D	1240	ILE	2.7
1	A	531	LEU	2.7
1	C	1300	SER	2.7
1	D	1318	LEU	2.7
1	A	45	TYR	2.7
1	A	942	PRO	2.6
1	B	730	CYS	2.6
1	D	556	PHE	2.6
1	B	992	PHE	2.6
1	D	557	PRO	2.6
1	D	1006	ILE	2.6
1	B	1317	ASN	2.6
1	C	480	LEU	2.6
1	C	701	VAL	2.6
1	D	280	VAL	2.6
1	C	546	SER	2.6
1	B	457	THR	2.6
1	D	45	TYR	2.6
1	D	458	ASP	2.6
1	B	477	CYS	2.6
1	C	739	VAL	2.6
1	B	536	THR	2.6
1	A	279	ASP	2.6
1	A	1006	ILE	2.6
1	B	866	ILE	2.6
1	D	481	ILE	2.6
1	D	470	VAL	2.6
1	B	1311	CYS	2.6
1	D	281	SER	2.6
1	A	967	THR	2.6
1	C	852	LYS	2.6
1	C	230	GLN	2.5
1	D	1286	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1295	ILE	2.5
1	B	280	VAL	2.5
1	D	703	VAL	2.5
1	D	864	ALA	2.5
1	A	455	THR	2.5
1	C	241	THR	2.5
1	D	420	SER	2.5
1	C	45	TYR	2.5
1	A	545	ILE	2.5
1	A	1318	LEU	2.5
1	B	397	LEU	2.5
1	C	992	PHE	2.5
1	D	424	PHE	2.5
1	A	938	LYS	2.5
1	C	733	GLN	2.5
1	B	858	ASN	2.5
1	D	448	VAL	2.5
1	C	720	GLU	2.5
1	D	499	GLU	2.5
1	B	480	LEU	2.5
1	A	296	VAL	2.5
1	B	369	ASN	2.5
1	C	731	ALA	2.5
1	A	730	CYS	2.4
1	A	1148	GLU	2.4
1	A	990	ASP	2.4
1	B	491	ASP	2.4
1	B	504	LEU	2.4
1	D	1334	VAL	2.4
1	B	1229	PRO	2.4
1	B	238	GLY	2.4
1	D	1197	ILE	2.4
1	D	531	LEU	2.4
1	D	496	MET	2.4
1	A	66	SER	2.4
1	A	497	ILE	2.4
1	A	959	ILE	2.4
1	D	735	LEU	2.4
1	D	334	TYR	2.4
1	D	952	TYR	2.4
1	D	522	PHE	2.4
1	B	1306	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	727	ALA	2.4
1	D	895	LYS	2.4
1	B	47	CYS	2.4
1	B	45	TYR	2.4
1	D	445	MET	2.4
1	C	723	ASN	2.4
1	A	398	ALA	2.4
1	A	1242	GLU	2.4
1	B	953	ARG	2.3
1	D	390	ILE	2.3
1	D	940	ARG	2.3
1	A	274	HIS	2.3
1	B	496	MET	2.3
1	D	863	ALA	2.3
1	B	1190	SER	2.3
1	C	722	GLY	2.3
1	C	940	ARG	2.3
1	D	859	GLY	2.3
1	A	708	GLN	2.3
1	C	523	LEU	2.3
1	D	404	ILE	2.3
1	D	503	LEU	2.3
1	C	571	ASP	2.3
1	A	257	MET	2.3
1	A	572	PHE	2.3
1	A	323	VAL	2.3
1	D	441	VAL	2.3
1	C	289	ALA	2.3
1	C	1297	ALA	2.3
1	B	1296	TRP	2.3
1	C	955	ILE	2.3
1	D	378	ILE	2.3
1	D	387	ILE	2.3
1	B	862	LYS	2.3
1	D	501	VAL	2.3
1	A	454	ASN	2.3
1	B	950	ASN	2.3
1	D	1229	PRO	2.3
1	C	418	ARG	2.3
1	C	1227	ARG	2.3
1	A	326	LEU	2.3
1	A	480	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	883	ILE	2.3
1	D	855	PHE	2.3
1	A	557	PRO	2.3
1	C	427	ALA	2.2
1	C	460	GLY	2.2
1	A	475	LYS	2.2
1	C	552	ILE	2.2
1	A	728	PHE	2.2
1	D	1195	VAL	2.2
1	D	1282	ALA	2.2
1	C	47	CYS	2.2
1	C	168	CYS	2.2
1	D	851	TYR	2.2
1	A	404	ILE	2.2
1	A	1332	ILE	2.2
1	C	900	ARG	2.2
1	D	449	PHE	2.2
1	A	857	ASN	2.2
1	A	952	TYR	2.2
1	B	527	TYR	2.2
1	C	938	LYS	2.2
1	C	326	LEU	2.2
1	D	494	GLY	2.2
1	C	865	ASP	2.2
1	A	449	PHE	2.2
1	A	1015	PRO	2.2
1	C	718	LYS	2.2
1	D	76	ALA	2.2
1	D	468	ALA	2.2
1	C	1231	GLN	2.2
1	D	1316	THR	2.2
1	A	47	CYS	2.2
1	A	523	LEU	2.2
1	A	1209	GLY	2.2
1	B	460	GLY	2.2
1	B	735	LEU	2.2
1	B	949	LEU	2.2
1	D	168	CYS	2.2
1	A	1227	ARG	2.2
1	B	556	PHE	2.2
1	D	572	PHE	2.2
1	D	1285	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	460	GLY	2.1
1	A	467	GLY	2.1
1	A	741	LEU	2.1
1	B	722	GLY	2.1
1	C	509	GLY	2.1
1	B	371	ILE	2.1
1	C	477	CYS	2.1
1	D	487	GLU	2.1
1	C	320	SER	2.1
1	D	1331	SER	2.1
1	A	1320	PRO	2.1
1	D	425	VAL	2.1
1	B	708	GLN	2.1
1	B	936	ALA	2.1
1	B	849	GLY	2.1
1	C	928	THR	2.1
1	C	625	ILE	2.1
1	D	456	ILE	2.1
1	D	726	GLU	2.1
1	B	555	ASP	2.1
1	C	1329	PRO	2.1
1	B	275	MET	2.1
1	D	525	MET	2.1
1	C	448	VAL	2.1
1	C	995	GLN	2.1
1	D	473	ALA	2.1
1	B	873	GLY	2.1
1	D	232	THR	2.1
1	D	958	THR	2.1
1	A	483	ARG	2.1
1	B	552	ILE	2.1
1	B	851	TYR	2.1
1	A	538	ASP	2.1
1	D	421	LYS	2.1
1	A	906	CYS	2.1
1	B	168	CYS	2.1
1	D	715	PRO	2.1
1	B	729	GLN	2.1
1	C	997	PHE	2.1
1	A	289	ALA	2.1
1	B	934	ALA	2.1
1	C	934	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	735	LEU	2.1
1	B	490	LEU	2.1
1	C	902	ARG	2.1
1	D	304	LEU	2.1
1	B	375	GLY	2.1
1	A	408	GLU	2.1
1	B	958	THR	2.1
1	B	1288	GLU	2.1
1	A	527	TYR	2.1
1	B	270	TYR	2.1
1	B	869	TYR	2.1
1	C	538	ASP	2.1
1	D	472	SER	2.1
1	B	169	PRO	2.1
1	A	496	MET	2.1
1	C	430	GLN	2.0
1	A	701	VAL	2.0
1	A	1319	VAL	2.0
1	C	1277	PHE	2.0
1	A	74	ALA	2.0
1	A	478	ARG	2.0
1	D	480	LEU	2.0
1	B	303	GLY	2.0
1	B	461	ILE	2.0
1	B	718	LYS	2.0
1	D	967	THR	2.0
1	D	942	PRO	2.0
1	D	856	MET	2.0
1	C	740	HIS	2.0
1	A	448	VAL	2.0
1	B	957	ARG	2.0
1	C	953	ARG	2.0
1	A	30	LEU	2.0
1	A	988	ALA	2.0
1	C	468	ALA	2.0
1	C	863	ALA	2.0
1	D	1310	ALA	2.0
1	A	499	GLU	2.0
1	B	1150	GLY	2.0
1	C	950	ASN	2.0
1	D	454	ASN	2.0
1	B	390	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	967	THR	2.0
1	C	580	ILE	2.0
1	B	1294	PRO	2.0
1	C	144	MET	2.0
1	D	956	ASP	2.0
1	A	463	TYR	2.0
1	D	527	TYR	2.0
1	D	711	SER	2.0

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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.

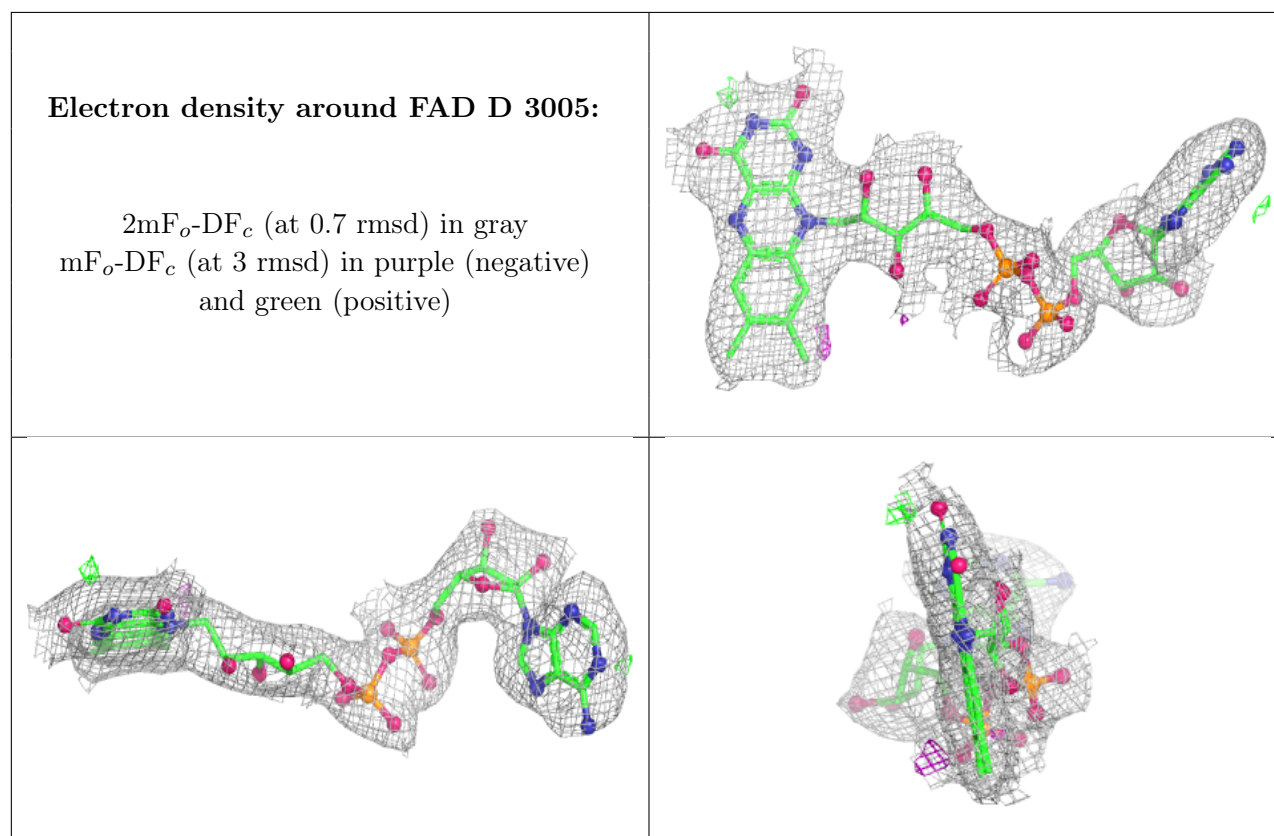
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	C	2337	1/1	0.86	0.12	50,50,50,50	0
2	NA	A	2337	1/1	0.90	0.09	26,26,26,26	0
2	NA	D	2337	1/1	0.93	0.08	17,17,17,17	0
6	FAD	D	3005	53/53	0.93	0.09	6,33,46,53	0
6	FAD	C	3005	53/53	0.94	0.10	9,31,49,50	0
6	FAD	B	3005	53/53	0.94	0.09	7,31,43,51	0
6	FAD	A	3005	53/53	0.95	0.08	9,28,45,49	0
4	MTE	B	3003	24/24	0.95	0.09	15,35,49,67	0
2	NA	B	2337	1/1	0.96	0.06	12,12,12,12	0
4	MTE	D	3003	24/24	0.96	0.08	13,33,49,53	0
4	MTE	A	3003	24/24	0.96	0.08	12,27,37,42	0
4	MTE	C	3003	24/24	0.97	0.08	7,32,46,61	0
5	MOS	D	3004	4/4	0.97	0.10	42,55,69,77	0
5	MOS	B	3004	4/4	0.98	0.09	42,55,69,77	0
3	FES	C	3001	4/4	0.98	0.04	24,24,31,39	0

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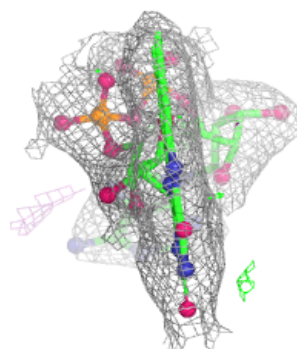
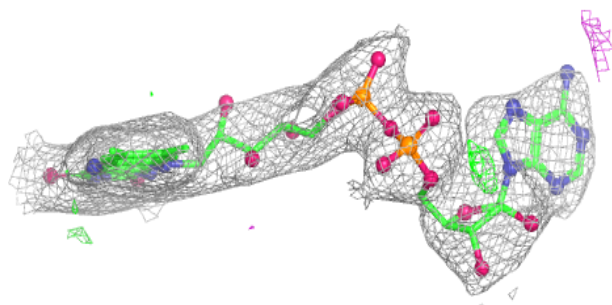
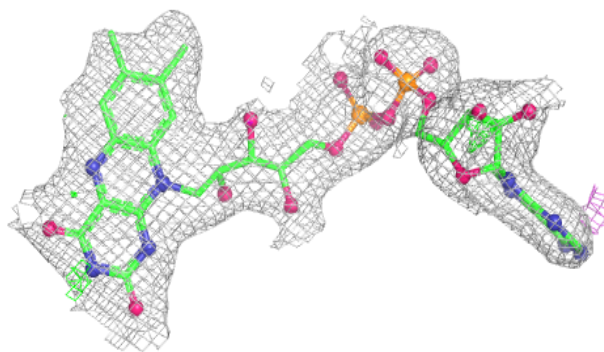
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FES	A	3001	4/4	0.99	0.03	19,20,23,26	0
5	MOS	A	3004	4/4	0.99	0.07	42,55,69,77	0
3	FES	C	3002	4/4	0.99	0.07	29,33,36,38	0
5	MOS	C	3004	4/4	0.99	0.09	42,55,69,77	0
3	FES	D	3001	4/4	0.99	0.02	15,23,23,26	0
3	FES	D	3002	4/4	0.99	0.03	15,24,25,41	0
3	FES	A	3002	4/4	0.99	0.04	16,23,33,38	0
3	FES	B	3001	4/4	0.99	0.02	7,20,22,26	0
3	FES	B	3002	4/4	0.99	0.03	20,21,34,38	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.

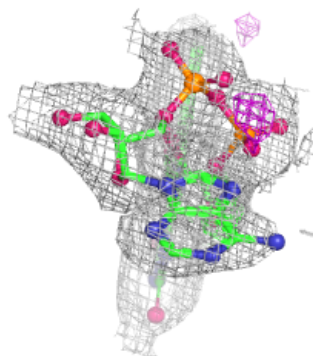
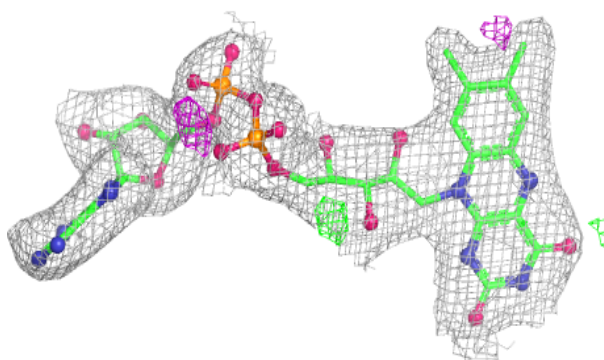


Electron density around FAD C 3005:

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

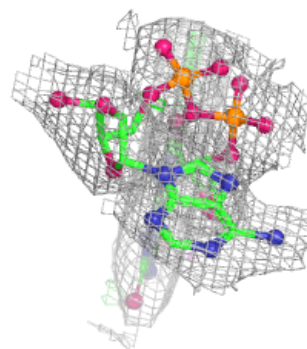
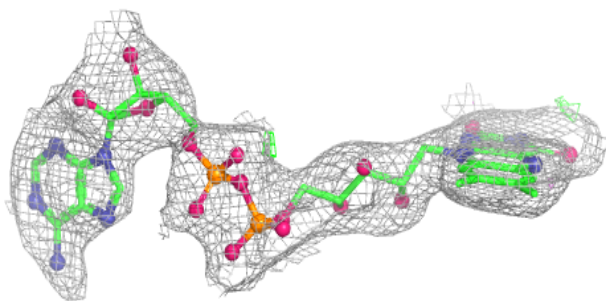
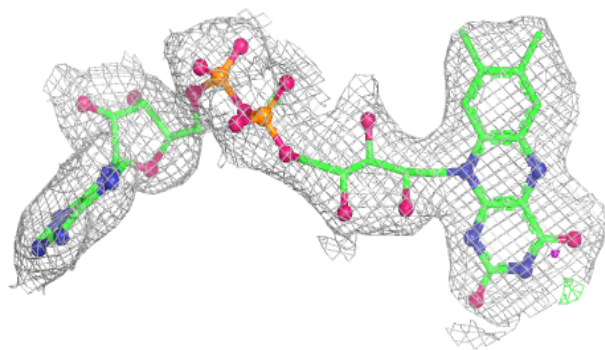
**Electron density around FAD B 3005:**

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



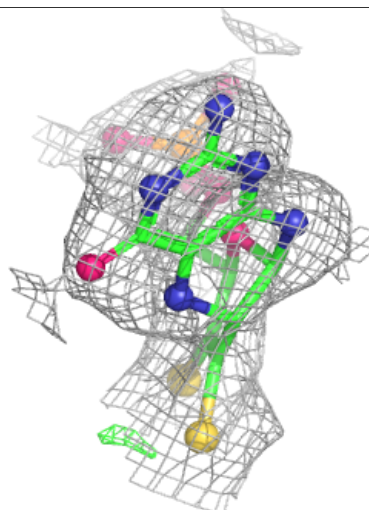
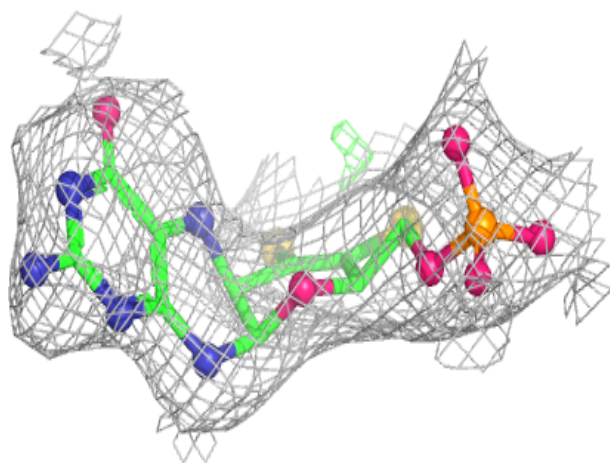
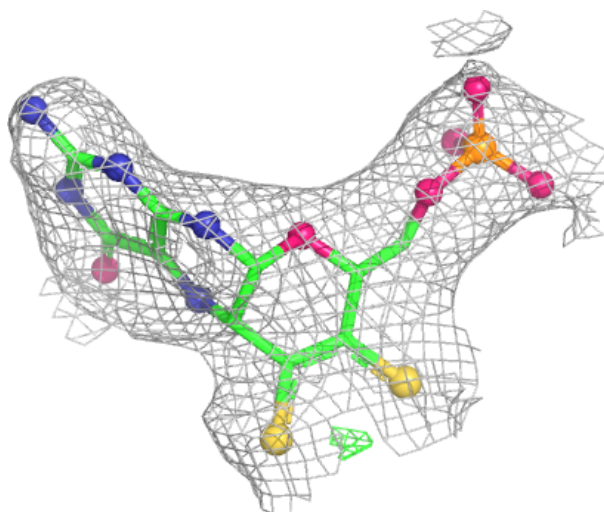
Electron density around FAD A 3005:

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



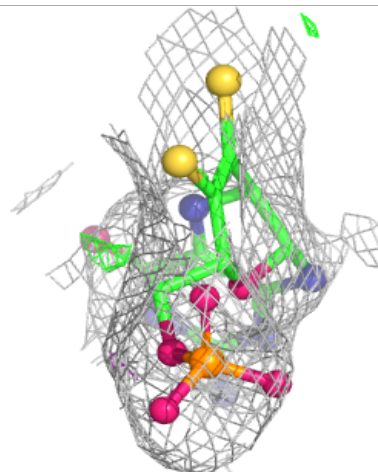
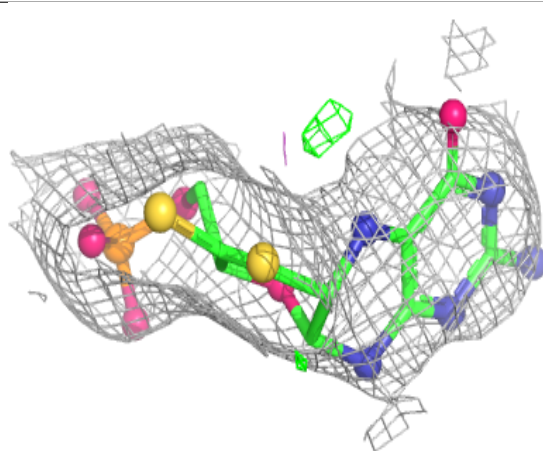
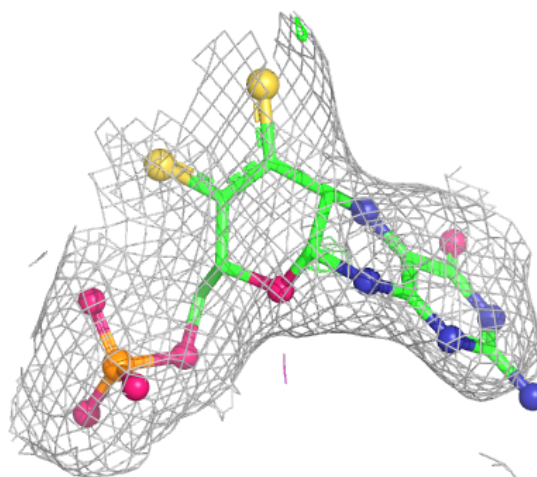
Electron density around MTE B 3003:

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



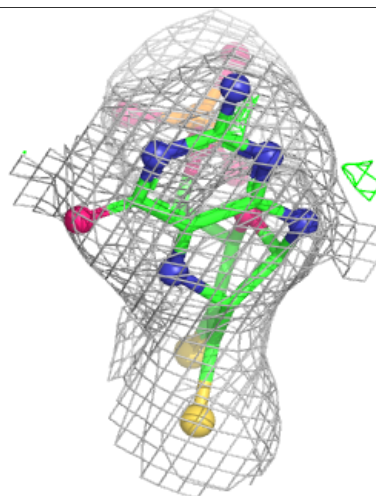
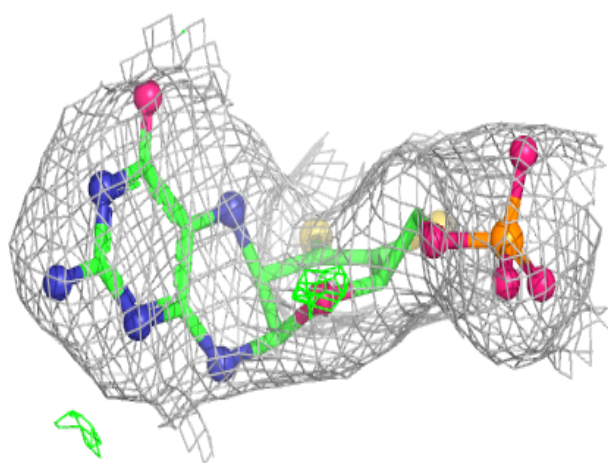
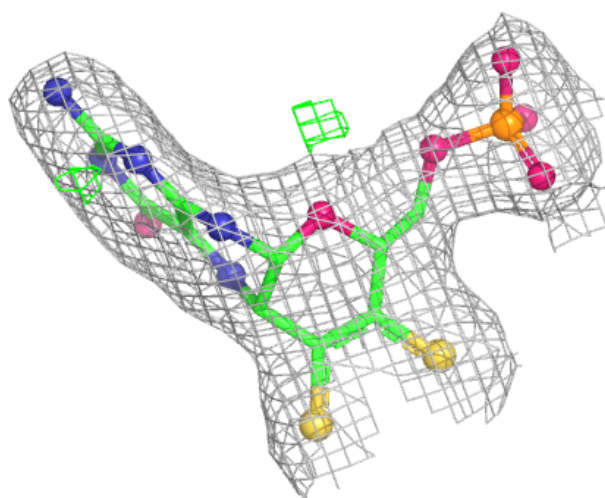
Electron density around MTE D 3003:

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



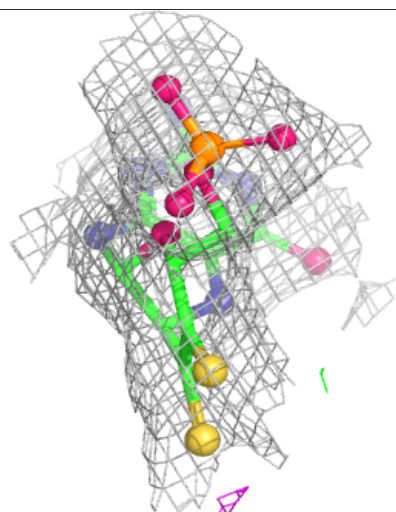
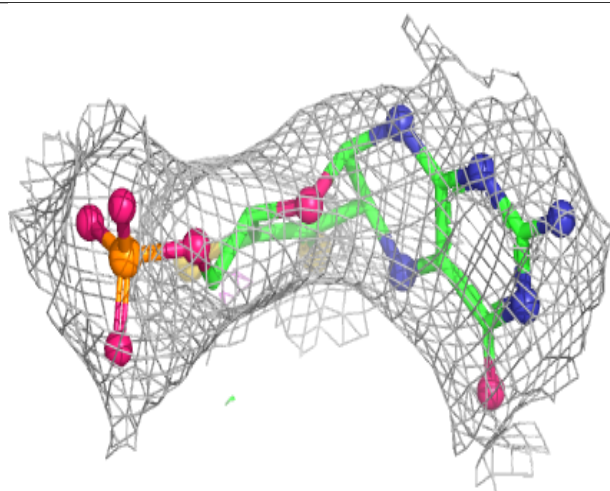
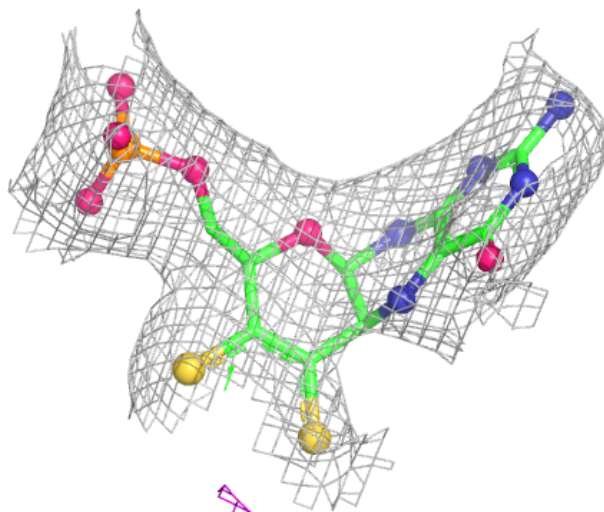
Electron density around MTE A 3003:

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



Electron density around MTE C 3003:

$2mF_o-DF_c$ (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.