Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2023 – 04:58 pm GMT

PDB ID	:	3ZYV
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:

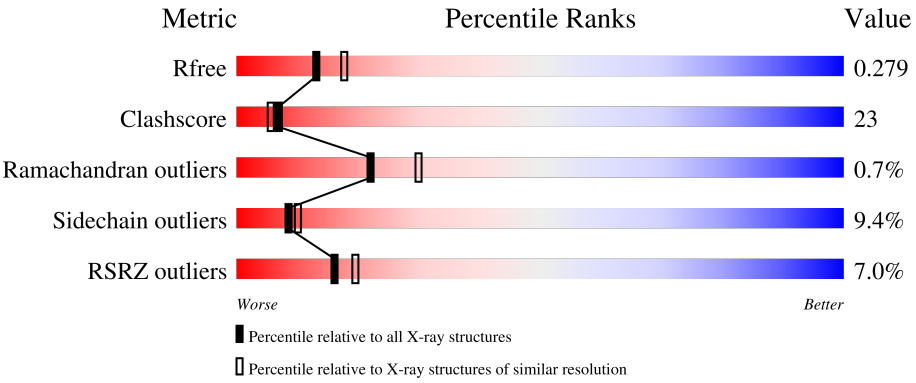
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	5% 58% 32% · 6%
1	B	1335	5% 57% 33% 5% 5%
1	C	1335	7% 59% 30% · 7%
1	D	1335	9% 58% 32% · 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	-
6	FAD	C	3005	-	-	X	-

2 Entry composition (i)

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.

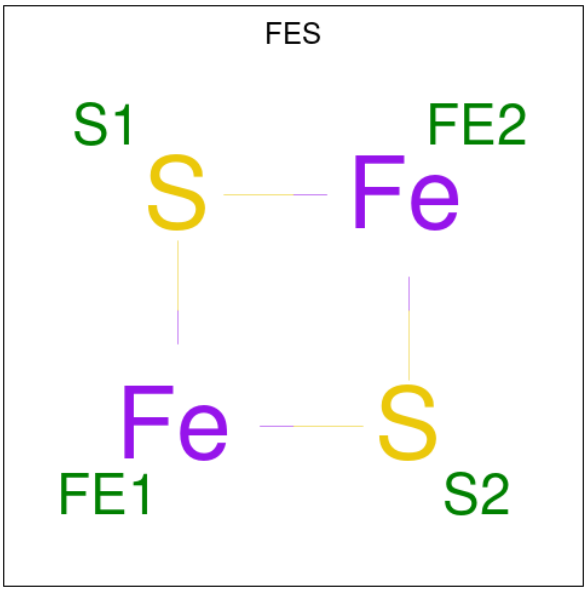
- Molecule 1 is a protein called AOX3.

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 (three-letter code: NA) (formula: Na).

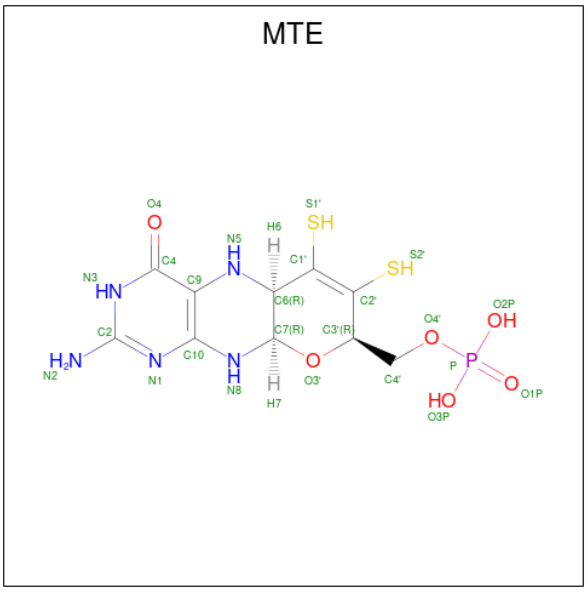
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



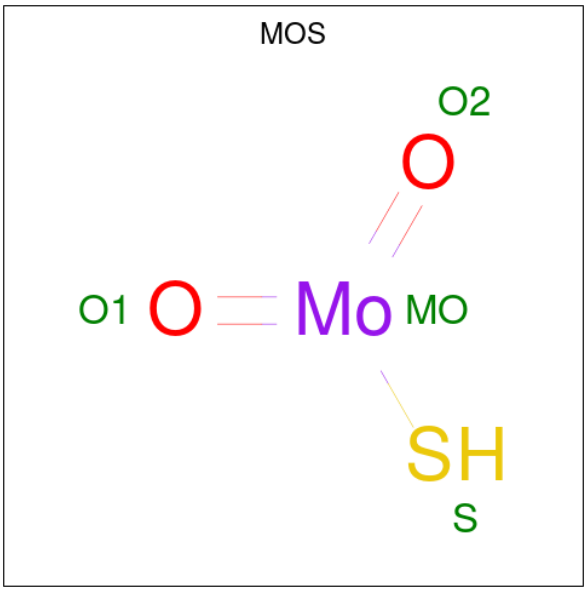
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 4 2 2	0	0
3	A	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	B	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	C	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0
3	D	1	Total Fe S 4 2 2	0	0

- 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 (three-letter code: MTE) (formula: $C_{10}H_{14}N_5O_6PS_2$).



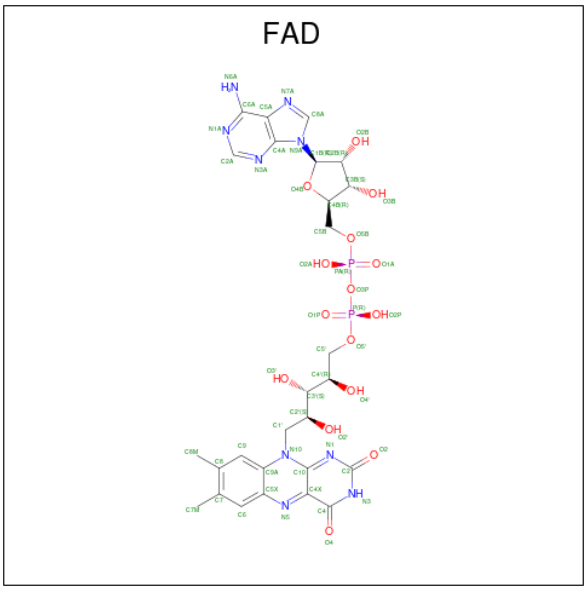
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	B	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	C	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		
4	D	1	Total	C	N	O	P	S	0	0
			24	10	5	6	1	2		

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: 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 (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	182	Total	O	0	0
			182	182		

Continued on next page...

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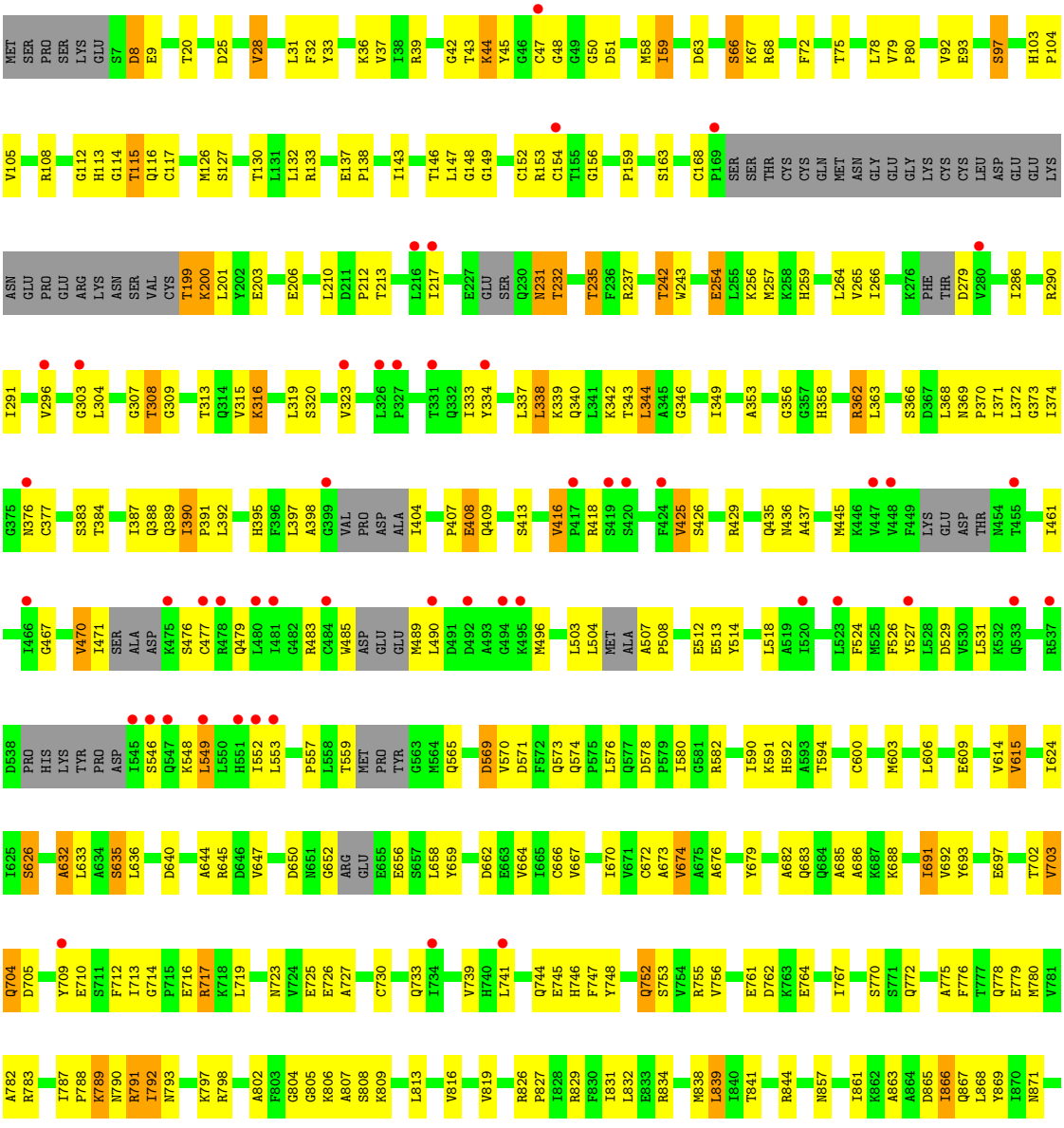
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	166	Total O 166 166	0	0
7	C	147	Total O 147 147	0	0
7	D	155	Total O 155 155	0	0

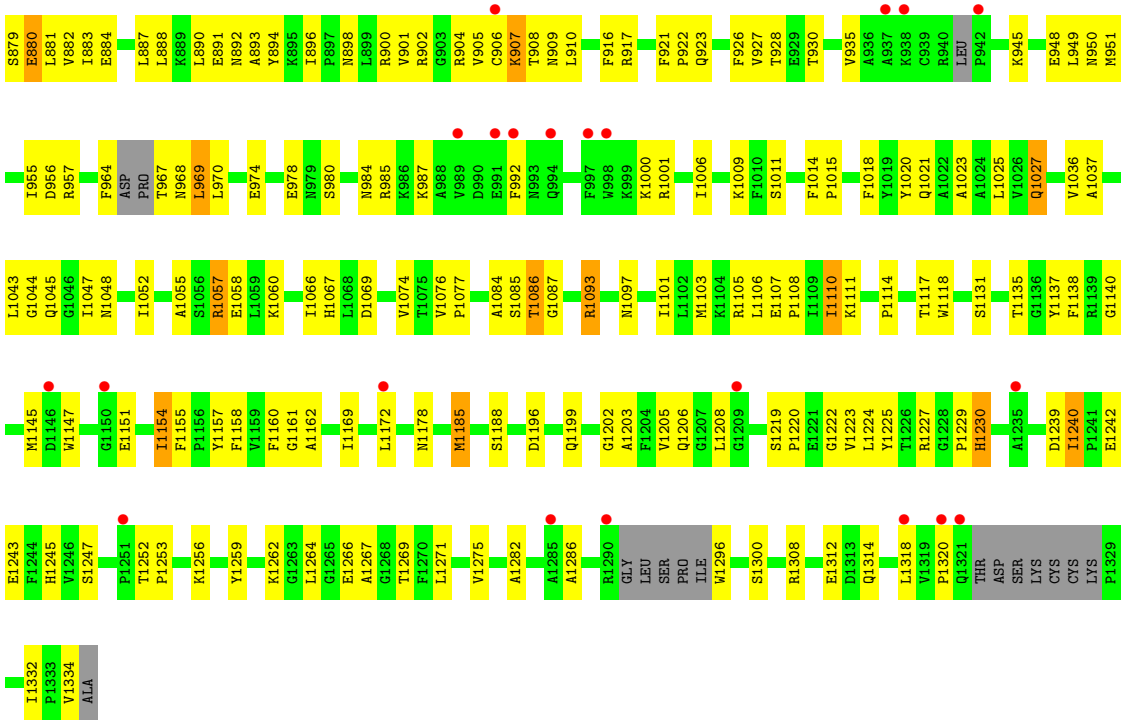
3 Residue-property plots (i)

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

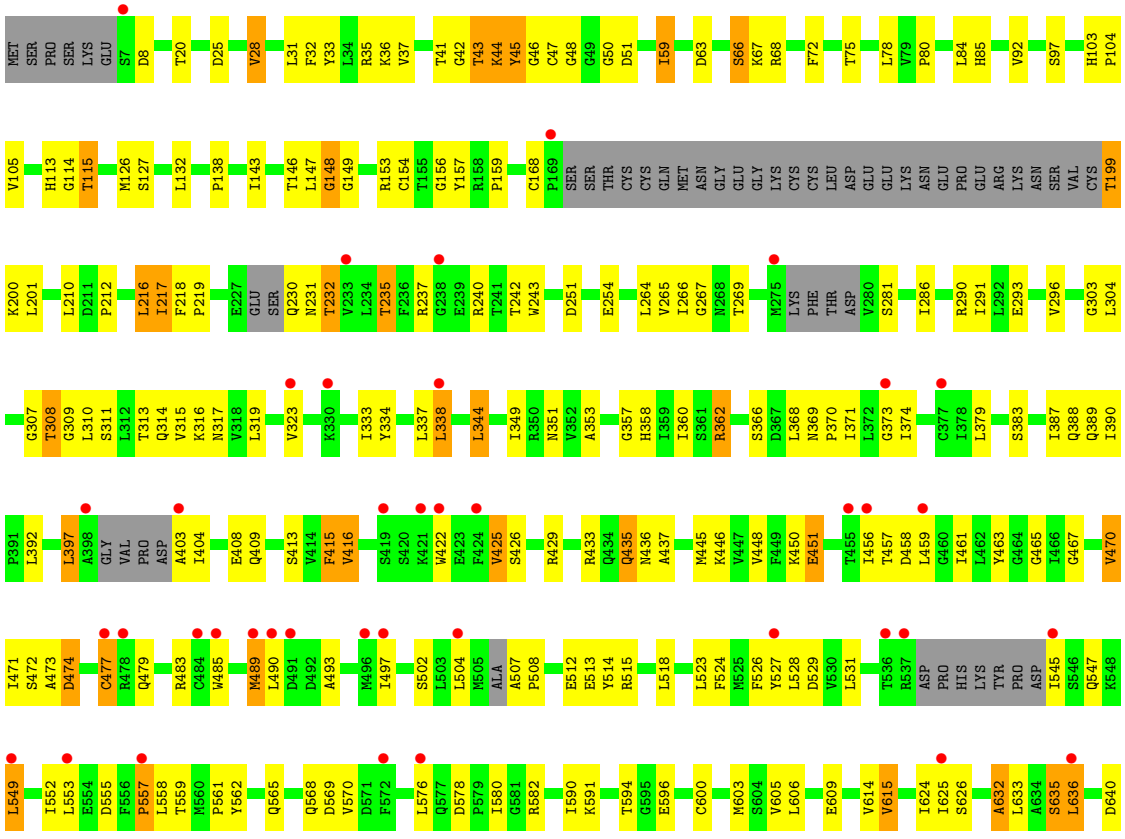
Chain A:

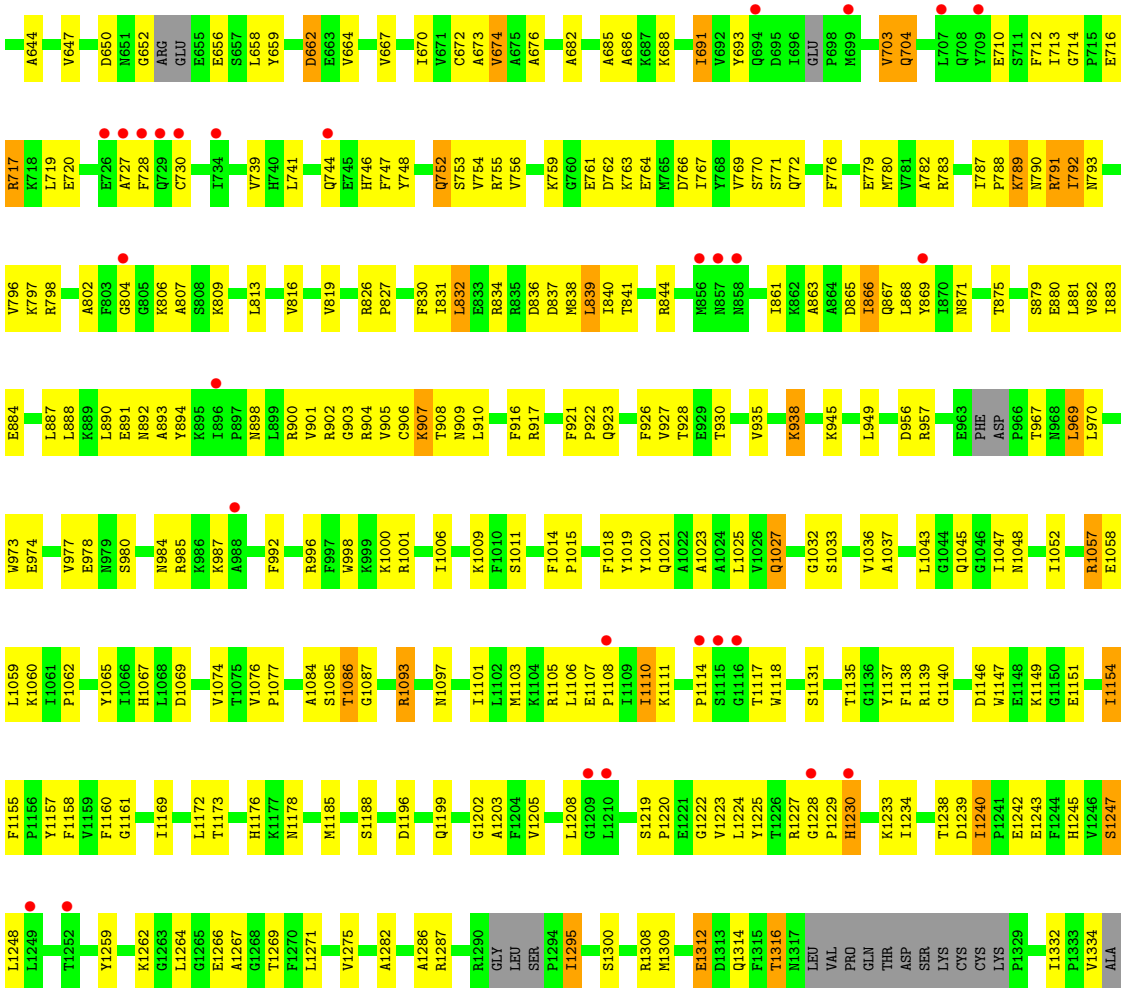




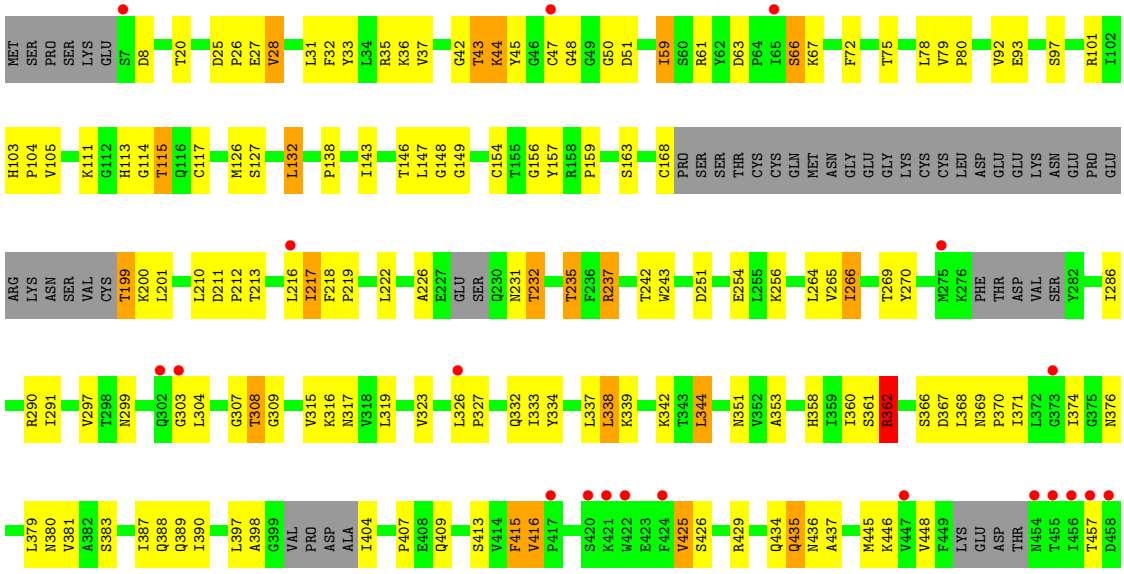
• Molecule 1: AOX3

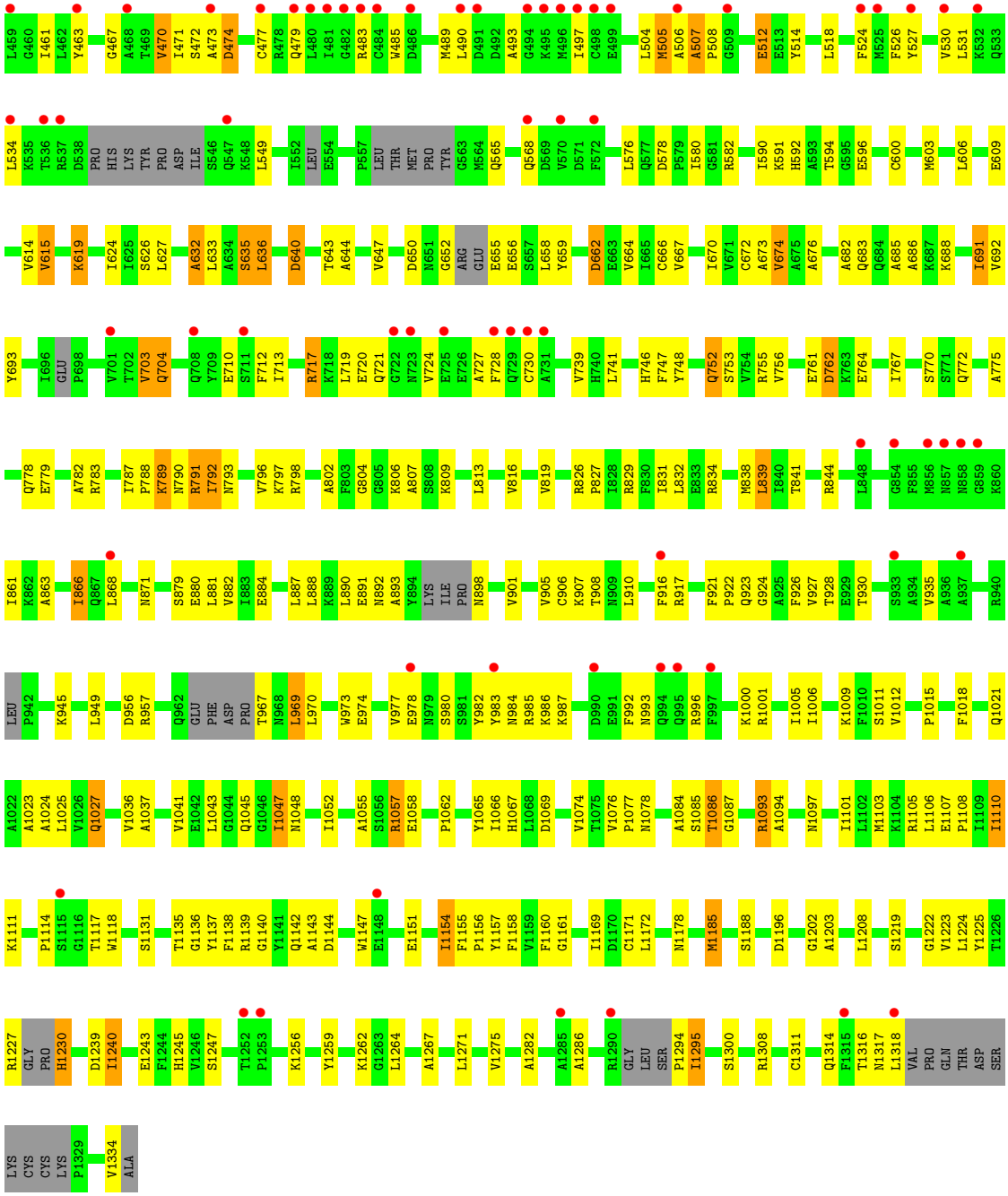
Chain B:



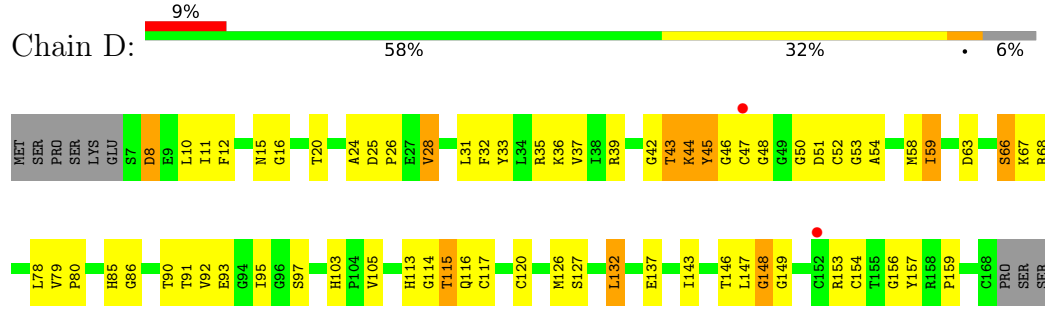


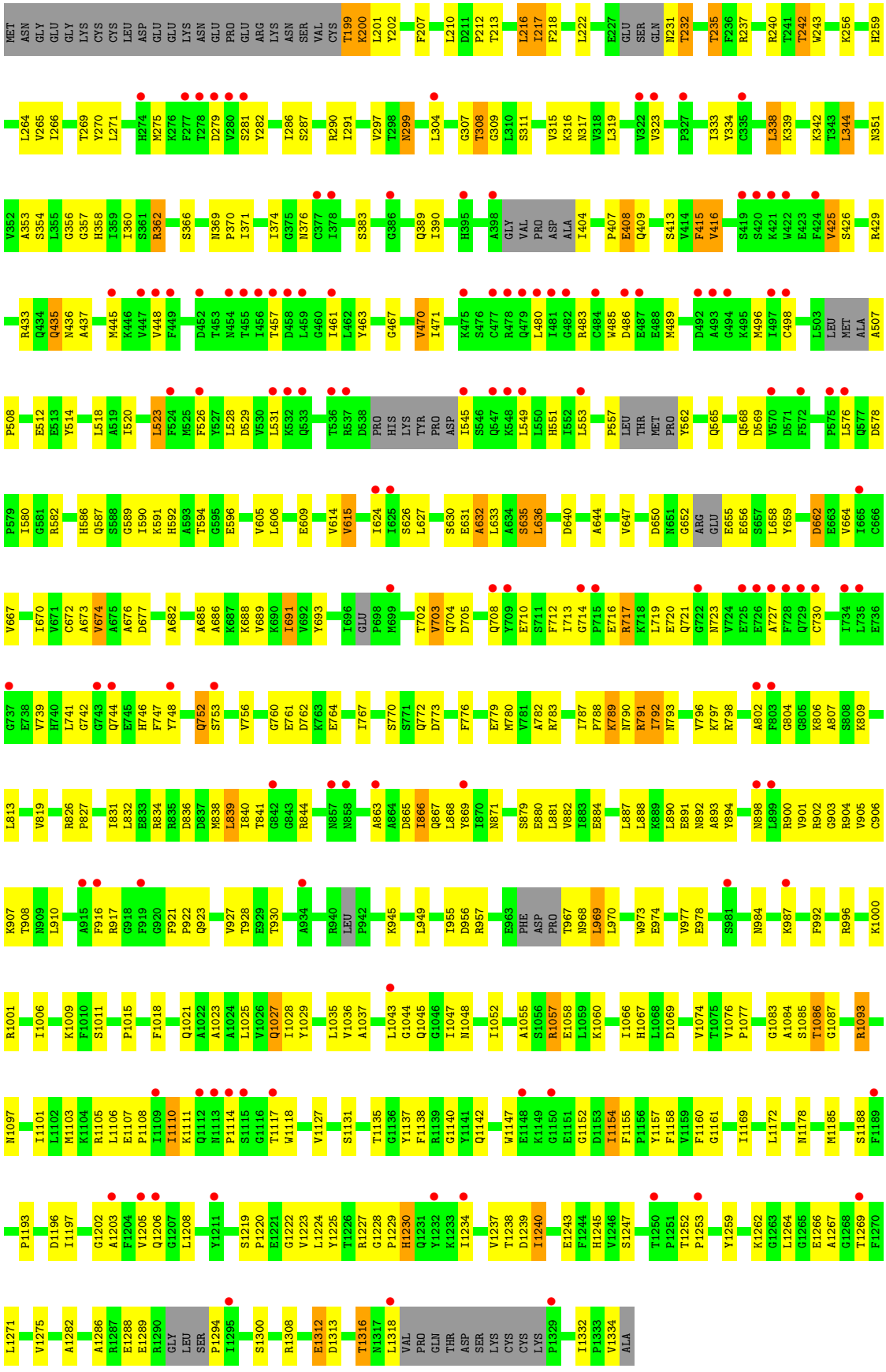
• Molecule 1: AOX3





• Molecule 1: AOX3




MET ASN GLY GLU GLY LYS CYS CYS LEU ASP GLU GLU LYS ASN GLU PRO GLU ARG LYS ASN SER VAL CYS T199 K200 L201 Y202 F207 L210 D211 P212 T213 L216 I217 F218 L222 E227 GLU SER GLN N231 T232 T235 F236 R237 R240 T241 T242 W243 K256 H259
L264 V265 I266 T269 Y270 L271 H274 M275 K276 F277 T278 D279 V280 S281 Y282 I286 S287 R290 I291 V297 T298 N299 L304 G307 T308 G309 L310 S311 V315 K316 N317 V318 L319 V322 V323 P327 I333 Y334 C335 L338 K339 K342 T343 L344 N351
V352 A353 S354 L355 G356 G357 H358 I359 I360 S361 R362 S366 N369 P370 I371 I374 G375 N376 C377 I378 S383 G386 Q389 I390 H395 A398 GLY VAL PRO ASP ALA I404 P407 E408 Q409 S413 V414 F415 V416 S419 S420 K421 W422 E423 F424 V425 S426 R429
R433 Q434 Q435 N436 A437 M445 K446 V447 V448 F449 D452 T453 N454 T455 I456 T457 D458 L459 G460 I461 L462 Y463 G467 V470 I471 K475 S476 C477 R478 Q479 L480 I481 G482 R483 C484 W485 D486 E487 E488 M489 D492 A493 G494 K495 M496 I497 C498 L503 LEU MET ALA A507
P508 E512 B513 Y514 L518 A519 I520 L523 F524 M525 F526 Y527 L528 D529 V530 L531 K532 Q533 T536 R537 D538 PRO HIS LYS TYR PRO ASP I545 S546 Q547 K548 L549 L550 H551 I552 L553 P557 LEU THR MET PRO Y562 Q565 Q568 D569 V570 D571 F572 P575 L576 Q577 D578
P579 I580 R581 R582 H586 Q587 S588 G589 I590 K591 H592 A593 T594 G595 E596 V605 L606 E609 V614 V615 I624 I625 S626 L627 S630 E631 A632 L633 A634 S635 L636 D640 A644 V647 D650 N651 G652 ARG GLU E655 E656 S657 L658 Y659 D662 E663 V664 I665 C666
V667 I670 V671 C672 A673 V674 A675 A676 D677 A682 A685 A686 K687 K688 V689 K690 I691 V692 Y693 I696 GLU P698 M699 T702 V703 Q704 D705 Q708 Y709 E710 S711 F712 I713 G714 P715 E716 R717 K718 L719 E720 Q721 G722 N723 V724 E725 E726 A727 F728 Q729 C730 I734 L735 E736
G737 E738 V739 H740 L741 G742 G743 Q744 E745 H746 F747 Y748 Q752 S753 V756 G760 E761 D762 K763 E764 I767 S770 S771 Q772 D773 F776 E779 M780 V781 A782 R783 I787 P788 K789 N790 R791 I792 N793 V796 K797 R798 A802 F803 G804 G805 K806 A807 S808 K809
L813 V819 R826 P827 I831 L832 E833 R834 R835 D836 D837 M838 L839 I840 T841 G842 G843 R844 N857 N858 A863 A864 D865 I866 Q867 L868 Y869 I870 N871 S879 E880 L881 V882 I883 E884 L887 L888 K889 L890 E891 N892 A893 Y894 N898 L899 R900 V901 R902 G903 R904 V905 C906
K907 T908 N909 L910 A915 F916 R917 G918 F919 Q920 F921 P922 Q923 V927 T928 E929 T930 A934 R940 LEU P942 K945 L949 I955 D956 R957 E963 PHE ASP PRO T967 N968 L969 L970 W973 E974 V977 E978 S981 N984 K987 F992 R996 K1000
R1001 I1006 K1009 F1010 S1011 P1015 F1018 Q1021 A1022 A1023 A1024 A1024 L1025 V1026 Q1027 I1028 Y1029 L1035 V1036 A1037 L1043 G1044 Q1045 G1046 I1047 N1048 I1052 A1055 S1056 R1057 E1058 L1059 K1060 I1066 H1067 L1068 D1069 V1074 T1075 V1076 P1077 G1083 A1084 S1085 T1086 G1087 R1093
N1097 I1101 L1102 M1103 K1104 R1105 L1106 E1107 P1108 I1109 I1110 K1111 Q1112 N1113 P1114 S1115 G1116 T1117 W1118 V1127 S1131 T1135 G1136 Y1137 F1138 R1139 G1140 Y1141 Q1142 W1147 E1148 K1149 G1150 E1151 G1152 D1153 I1154 F1155 P1156 Y1157 F1158 V1159 F1160 G1161 I1169 L1172 N1178 M1185 S1188 F1189
P1193 D1196 I1197 G1202 A1203 F1204 V1205 Q1206 G1207 L1208 Y1211 S1219 P1220 E1221 G1222 V1223 L1224 Y1225 T1226 R1227 G1228 P1229 H1230 Q1231 Y1232 K1233 I1234 V1237 T1238 D1239 I1240 E1243 F1244 H1245 V1246 S1247 T1250 P1251 T1252 P1253 Y1259 K1262 G1263 L1264 G1265 E1266 A1267 G1268 T1269 F1270
L1271 V1275 A1282 A1286 R1287 E1288 E1289 R1290 GLY LEU SER P1294 I1295 S1300 R1308 E1312 D1313 T1316 N1317 L1318 VAL PRO GLN THR ASP SER LYS CYS CYS LYS P1329 I1332 P1333 V1334 ALA

4 Data and refinement statistics (i)

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 – 2.55	Depositor EDS
% Data completeness (in resolution range)	75.0 (49.91-2.54) 75.0 (49.91-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.285 0.250 , 0.279	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)	0.34 , 66.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: FES, MTE, MOS, NA, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.31	0/9482	0.50	1/12869 (0.0%)
1	B	0.32	0/9650	0.50	2/13097 (0.0%)
1	C	0.31	0/9398	0.51	1/12757 (0.0%)
1	D	0.31	0/9460	0.49	0/12852
All	All	0.31	0/37990	0.50	4/51575 (0.0%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	619	LYS	CB-CG-CD	7.44	130.95	111.60
1	A	697	GLU	C-N-CD	-6.60	106.07	120.60
1	B	558	LEU	N-CA-C	-6.30	93.99	111.00
1	B	561	PRO	N-CA-CB	5.06	109.37	103.30

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	438	0
1	B	9471	0	9271	446	0
1	C	9231	0	8962	414	0
1	D	9289	0	8958	438	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
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	21	0
6	D	53	0	31	15	0
7	A	182	0	0	93	0
7	B	166	0	0	65	0
7	C	147	0	0	57	0
7	D	155	0	0	90	0
All	All	38315	0	36401	1701	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 23.

All (1701) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:269:THR:HG1	6:D:3005:FAD:HO3'	0.90	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: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: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:B:769:VAL:C	7:B:2115:HOH:O	2.19	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:D:269:THR:OG1	6:D:3005:FAD:O3'	1.81	0.79
1:A:752:GLN:NE2	7:A:2128:HOH:O	1.91	0.79
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:A:92:VAL:HA	1:A:126:MET:HE1	1.65	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:269:THR:HB	6:B:3005:FAD:HM81	1.65	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:THR:O	7:D:2057:HOH:O	2.01	0.77
1:C:92:VAL:HA	1:C:126:MET:HE1	1.65	0.77
1:D:358:HIS:HE2	1:D:366:SER:HG	1.32	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: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:C:983:TYR:C	7:C:2114:HOH:O	2.22	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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLN:OE1	7:A:2120:HOH:O	2.06	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:B:314:GLN:CD	7:B:2052:HOH:O	2.27	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:31:LEU:CD2	1:C:45:TYR:HB3	2.19	0.72
1:C:1161:GLY:HA3	1:C:1185:MET:HE2	1.71	0.72
1:D:92:VAL:HA	1:D:126:MET:HE1	1.70	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
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: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:B:1161:GLY:HA3	1:B:1185:MET:HE2	1.71	0.71
1:D:1161:GLY:HA3	1:D:1185:MET:HE2	1.71	0.71
1:C:923:GLN:O	7:C:2112:HOH:O	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:MET:HG2	1:D:461:ILE:HG23	1.71	0.71
1:C:269:THR:OG1	6:C:3005:FAD:H5'2	1.90	0.70
1:B:938:LYS:HZ1	1:B:1295:ILE:HD13	1.55	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: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
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:A:1161:GLY:HA3	1:A:1185:MET:HE2	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:D:655:GLU:CD	7:D:2096:HOH:O	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:506:ALA:HB1	1:C:512:GLU:CD	2.13	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: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
1:B:1036:VAL:O	7:B:2142:HOH:O	2.12	0.67
1:B:1262:LYS:NZ	7:B:2155:HOH:O	2.27	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: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:D:1093:ARG:HH11	1:D:1093:ARG:HG2	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:92:VAL:HA	1:B:126:MET:HE1	1.78	0.65
1:A:339:LYS:O	7:A:2062:HOH:O	2.15	0.65
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: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:948:GLU:C	7:A:2143:HOH:O	2.35	0.64
1:A:987:LYS:CE	7:A:2150:HOH:O	2.46	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:A:548:LYS:N	7:A:2086:HOH:O	2.31	0.63
1:B:415:PHE:C	1:B:415:PHE:HD1	2.02	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:63:ASP:N	7:B:2018:HOH:O	2.32	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
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:C:1136:GLY:C	7:C:2119:HOH:O	2.37	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:490:LEU:C	1:A:490:LEU:HD23	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:490:LEU:HD23	1:C:490:LEU:C	2.21	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:C:719:LEU:HD11	1:C:888:LEU:HD23	1.83	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:B:490:LEU:C	1:B:490:LEU:HD23	2.21	0.61
1:A:25:ASP:O	1:A:28:VAL:HG13	2.01	0.61
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:B:415:PHE:C	1:B:415:PHE:CD1	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:415:PHE:C	1:D:415:PHE:CD1	2.74	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
1:A:1103:MET:HE2	1:A:1103:MET:HA	1.85	0.59
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:415:PHE:CD1	1:C:415:PHE:C	2.75	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: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: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:D:15:ASN:CG	7:D:2004:HOH:O	2.42	0.58
1:A:741:LEU:HD11	1:A:926:PHE:CD2	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: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:358:HIS:NE2	1:C:366:SER:OG	2.35	0.58
1:C:703:VAL:HG12	1:C:1334:VAL:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:VAL:O	1:D:667:VAL:HG22	2.02	0.58
1:B:545:ILE:HG23	1:B:545:ILE:O	2.04	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:D:1103:MET:HE1	1:D:1118:TRP:HZ3	1.68	0.58
1:A:47:CYS:SG	1:A:48:GLY:N	2.74	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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:344:LEU:HD12	1:B:344:LEU:C	2.25	0.56
1:B:358:HIS:NE2	1:B:366:SER:OG	2.36	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
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:344:LEU:C	1:D:344:LEU:HD12	2.26	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: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: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:B:1103:MET:HE1	1:B:1118:TRP:HZ3	1.70	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:C:344:LEU:C	1:C:344:LEU:HD12	2.27	0.56
1:C:415:PHE:C	1:C:415:PHE:HD1	2.10	0.56
1:D:647:VAL:HG23	1:D:647:VAL:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1103:MET:HE2	1:B:1103:MET:HA	1.89	0.55
1:C:27:GLU:HG3	7:C:2004:HOH:O	2.07	0.55
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:92:VAL:HA	1:B:126:MET:CE	2.37	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:1103:MET:HE1	1:C:1118:TRP:HZ3	1.71	0.55
1:A:344:LEU:C	1:A:344:LEU:HD12	2.28	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1103:MET:HA	1:C:1103:MET:HE2	1.89	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:C:578:ASP:C	1:C:578:ASP:OD1	2.45	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: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: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
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:A:387:ILE:HG22	1:A:388:GLN:N	2.22	0.54
1:C:265:VAL:HG13	1:C:265:VAL:O	2.08	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: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:251:ASP:CG	7:C:2043:HOH:O	2.44	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:415:PHE:C	1:D:415:PHE:HD1	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1103:MET:HE1	1:A:1118:TRP:HZ3	1.72	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: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:1220:PRO:HA	1:D:1332:ILE:HD13	1.90	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
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:D:265:VAL:HG13	1:D:265:VAL:O	2.08	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: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:D:578:ASP:OD1	1:D:578:ASP:C	2.46	0.53
1:A:546:SER:CB	7:A:2086:HOH:O	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:916:PHE:O	1:A:917:ARG:C	2.48	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:C:1103:MET:HA	1:C:1103:MET:CE	2.40	0.52
1:D:270:TYR:HB3	6:D:3005:FAD:O1A	2.09	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1110:ILE:O	1:A:1110:ILE:HG13	2.09	0.52
1:B:371:ILE:HA	1:B:374:ILE:HG22	1.92	0.51
1:B:450:LYS:O	1:B:451:GLU:C	2.49	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: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:578:ASP:OD1	1:B:578:ASP:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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: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:578:ASP:C	1:A:578:ASP:OD1	2.49	0.51
1:A:790:ASN:OD1	1:A:791:ARG:HD3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:92:VAL:HA	1:A:126:MET:CE	2.38	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
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:B:770:SER:C	7:B:2115:HOH:O	2.39	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: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:D:1103:MET:HA	1:D:1103:MET:CE	2.42	0.50
1:A:1077:PRO:CG	1:B:1027:GLN:HG3	2.39	0.50
1:B:358:HIS:HE2	1:B:366:SER:HG	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:B:1103:MET:HA	1:B:1103:MET:CE	2.42	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
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: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:269:THR:HB	6:C:3005:FAD:HM81	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:916:PHE:O	1:C:917:ARG:C	2.49	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
1:A:1314:GLN:CD	1:A:1314:GLN:H	2.15	0.49
1:B:472:SER:C	1:B:474:ASP:H	2.16	0.49
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:SER:O	1:B:67:LYS:HB2	2.12	0.49
1:C:358:HIS:HE2	1:C:366:SER:HG	1.61	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
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:D:199:THR:OG1	1:D:200:LYS:N	2.46	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1103:MET:HA	1:D:1103:MET:HE2	1.96	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: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
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: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:514:TYR:HA	1:B:1309:MET:HE3	1.96	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: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:C:216:LEU:HD12	1:C:216:LEU:H	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:308:THR:HG22	1:B:309:GLY:N	2.27	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:B:199:THR:OG1	1:B:200:LYS:N	2.46	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:D:916:PHE:O	1:D:917:ARG:C	2.52	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:764:GLU:CD	7:A:2130:HOH:O	2.53	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
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:967:THR:C	7:B:2131:HOH:O	2.52	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:B:1314:GLN:H	1:B:1314:GLN:CD	2.18	0.47
1:C:374:ILE:HG13	1:C:446:LYS:HB3	1.96	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:713:ILE:CG1	1:D:907:LYS:HB3	2.30	0.47
1:D:776:PHE:CE1	1:D:780:MET:HE2	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:888:LEU:HD13	1:A:1154:ILE:CD1	2.45	0.46
1:B:473:ALA:O	1:B:474:ASP:C	2.53	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: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:916:PHE:C	5:B:3004:MOS:S	2.94	0.46
1:B:1146:ASP:OD2	1:B:1149:LYS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1067:HIS:CE1	1:D:764:GLU:OE2	2.69	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:506:ALA:CB	1:C:512:GLU:CD	2.81	0.46
1:C:890:LEU:HD12	1:C:891:GLU:N	2.30	0.46
1:D:871:ASN:HD21	1:D:908:THR:HG21	1.81	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: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: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: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:C:1314:GLN:CD	1:C:1314:GLN:H	2.18	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: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:B:1014:PHE:O	1:B:1020:TYR:OH	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:A:916:PHE:C	5:A:3004:MOS:S	2.95	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:D:433:ARG:NH1	1:D:1234:ILE:O	2.49	0.45
1:A:58:MET:CG	7:A:2015:HOH:O	2.54	0.45
1:C:103:HIS:CG	1:C:104:PRO:HD2	2.51	0.45
1:C:924:GLY:C	7:C:2112:HOH:O	2.53	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:HIS:C	1:A:115:THR:H	2.20	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: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: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:691:ILE:HD11	1:B:693:TYR:CE1	2.52	0.45
1:C:113:HIS:C	1:C:115:THR:H	2.20	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:156:GLY:O	1:B:157:TYR:HB2	2.17	0.45
1:D:58:MET:N	7:D:2012:HOH:O	2.49	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: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:776:PHE:CE1	1:B:780:MET:HE2	2.52	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:VAL:O	1:A:819:VAL:HG22	2.17	0.44
1:B:369:ASN:HB2	1:B:370:PRO:HD3	1.99	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:D:916:PHE:C	5:D:3004:MOS:S	2.96	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: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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:916:PHE:C	5:C:3004:MOS:S	2.96	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:217:ILE:O	1:C:218:PHE:C	2.56	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: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: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
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:D:147:LEU:C	1:D:149:GLY:N	2.72	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:505:MET:HE3	1:C:512:GLU:HG2	2.00	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: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:969:LEU:HA	1:C:1160:PHE:HB3	2.00	0.43
1:C:1036:VAL:HG12	1:C:1037:ALA:N	2.34	0.43
1:C:1334:VAL:O	1:C:1334:VAL:HG12	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:PHE:O	1:B:917:ARG:C	2.56	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:C:472:SER:C	1:C:474:ASP:H	2.21	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: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:B:562:TYR:CD1	1:B:562:TYR:C	2.92	0.43
1:B:938:LYS:NZ	1:B:1295:ILE:HD13	2.31	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: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: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:485:TRP:CE2	7:C:2066:HOH:O	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:217:ILE:O	1:B:218:PHE:C	2.57	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: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:D:333:ILE:HA	1:D:425:VAL:HG21	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:893:ALA:HB1	1:A:969:LEU:HD11	2.01	0.42
1:B:113:HIS:C	1:B:115:THR:H	2.22	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:11:ILE:C	7:D:2002:HOH:O	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:868:LEU:HD12	1:A:887:LEU:CD2	2.49	0.42
1:C:632:ALA:O	1:C:633:LEU:C	2.58	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:776:PHE:CE1	1:A:780:MET:HE2	2.55	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:299:ASN:O	1:D:299:ASN:CG	2.58	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:490:LEU:C	1:A:490:LEU:CD2	2.88	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
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:1085:SER:OG	1:A:1266:GLU:HG3	2.19	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: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:632:ALA:O	1:A:633:LEU:C	2.57	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1055:ALA:CB	1:A:1066:ILE:HD13	2.50	0.41
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
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:113:HIS:C	1:D:115:THR:H	2.23	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:709:TYR:O	1:A:710:GLU:C	2.59	0.41
1:A:1105:ARG:NH1	1:A:1131:SER:O	2.53	0.41
1:B:1243:GLU:HG2	1:B:1245:HIS:NE2	2.35	0.41
1:B:1332:ILE:HG13	1:B:1332:ILE:O	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:217:ILE:O	1:D:218:PHE:C	2.59	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:755:ARG:HG2	1:C:829:ARG:HG3	2.01	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: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: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: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: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:490:LEU:C	1:B:490:LEU:CD2	2.89	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:361:SER:O	1:C:362:ARG:C	2.58	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:1035:LEU:CD1	7:D:2134:HOH:O	2.68	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: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:346:GLY:C	7:A:2064:HOH:O	2.59	0.41
1:A:395:HIS:C	1:A:397:LEU:N	2.74	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:880:GLU:CD	1:A:880:GLU:N	2.74	0.41
1:A:1014:PHE:O	1:A:1020:TYR:OH	2.31	0.41
1:A:1107:GLU:HB3	1:A:1108:PRO:CD	2.50	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: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:C:1294:PRO:O	1:C:1295:ILE:C	2.59	0.41
1:D:51:ASP:OD1	1:D:51:ASP:O	2.39	0.41
1:D:291:ILE:N	1:D:291:ILE:CD1	2.84	0.41
1:D:627:LEU:HD13	1:D:627:LEU:C	2.41	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:84:LEU:O	1:B:85:HIS:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:275:MET:CG	1:D:282:TYR:HE2	2.34	0.41
1:D:632:ALA:O	1:D:633:LEU:C	2.59	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:210:LEU:O	1:A:212:PRO:HD3	2.21	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: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:147:LEU:C	1:A:149:GLY:N	2.74	0.40
1:A:203:GLU:O	1:A:206:GLU:HG2	2.21	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:D:147:LEU:O	1:D:148:GLY:C	2.60	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:627:LEU:C	1:C:627:LEU:HD13	2.42	0.40
1:C:775:ALA:O	1:C:778:GLN:HB3	2.21	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: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:147:LEU:C	1:D:149:GLY:H	2.24	0.40
1:D:311:SER:O	1:D:315:VAL:HG23	2.21	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:B:147:LEU:C	1:B:149:GLY:N	2.74	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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1221/1335 (92%)	1123 (92%)	89 (7%)	9 (1%)	22	30
1	B	1238/1335 (93%)	1137 (92%)	93 (8%)	8 (1%)	25	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	1210/1335 (91%)	1111 (92%)	88 (7%)	11 (1%)	17 24
1	D	1231/1335 (92%)	1120 (91%)	104 (8%)	7 (1%)	25 34
All	All	4900/5340 (92%)	4491 (92%)	374 (8%)	35 (1%)	22 30

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
1	C	148	GLY

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Mol	Chain	Res	Type
1	C	796	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	958/1129 (85%)	869 (91%)	89 (9%)	9 10
1	B	988/1129 (88%)	891 (90%)	97 (10%)	8 9
1	C	948/1129 (84%)	862 (91%)	86 (9%)	9 11
1	D	941/1129 (83%)	854 (91%)	87 (9%)	9 11
All	All	3835/4516 (85%)	3476 (91%)	359 (9%)	8 10

All (359) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	20	THR
1	A	28	VAL
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	117	CYS
1	A	127	SER
1	A	132	LEU
1	A	163	SER
1	A	199	THR
1	A	200	LYS
1	A	217	ILE
1	A	231	ASN
1	A	232	THR
1	A	235	THR
1	A	237	ARG

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Mol	Chain	Res	Type
1	A	242	THR
1	A	254	GLU
1	A	266	ILE
1	A	279	ASP
1	A	296	VAL
1	A	304	LEU
1	A	308	THR
1	A	316	LYS
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	470	VAL
1	A	477	CYS
1	A	479	GLN
1	A	512	GLU
1	A	531	LEU
1	A	549	LEU
1	A	569	ASP
1	A	615	VAL
1	A	626	SER
1	A	635	SER
1	A	636	LEU
1	A	640	ASP
1	A	658	LEU
1	A	666	CYS
1	A	670	ILE
1	A	674	VAL
1	A	691	ILE
1	A	703	VAL
1	A	704	GLN
1	A	717	ARG
1	A	726	GLU
1	A	747	PHE
1	A	748	TYR
1	A	752	GLN

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Mol	Chain	Res	Type
1	A	789	LYS
1	A	791	ARG
1	A	792	ILE
1	A	832	LEU
1	A	839	LEU
1	A	866	ILE
1	A	880	GLU
1	A	881	LEU
1	A	907	LYS
1	A	969	LEU
1	A	978	GLU
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	1110	ILE
1	A	1117	THR
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	1312	GLU
1	B	8	ASP
1	B	20	THR
1	B	28	VAL
1	B	43	THR
1	B	44	LYS
1	B	45	TYR
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	199	THR
1	B	216	LEU
1	B	217	ILE

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Mol	Chain	Res	Type
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	296	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	435	GLN
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	523	LEU
1	B	531	LEU
1	B	549	LEU
1	B	569	ASP
1	B	605	VAL
1	B	615	VAL
1	B	626	SER
1	B	635	SER
1	B	636	LEU
1	B	640	ASP
1	B	658	LEU
1	B	670	ILE

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Mol	Chain	Res	Type
1	B	674	VAL
1	B	691	ILE
1	B	703	VAL
1	B	704	GLN
1	B	717	ARG
1	B	720	GLU
1	B	728	PHE
1	B	747	PHE
1	B	748	TYR
1	B	752	GLN
1	B	789	LYS
1	B	791	ARG
1	B	792	ILE
1	B	832	LEU
1	B	839	LEU
1	B	866	ILE
1	B	880	GLU
1	B	881	LEU
1	B	907	LYS
1	B	938	LYS
1	B	969	LEU
1	B	978	GLU
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	1110	ILE
1	B	1117	THR
1	B	1139	ARG
1	B	1151	GLU
1	B	1154	ILE
1	B	1224	LEU
1	B	1230	HIS
1	B	1240	ILE
1	B	1247	SER
1	B	1295	ILE
1	B	1312	GLU
1	B	1316	THR
1	C	8	ASP
1	C	20	THR

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Mol	Chain	Res	Type
1	C	28	VAL
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	117	CYS
1	C	127	SER
1	C	132	LEU
1	C	163	SER
1	C	199	THR
1	C	217	ILE
1	C	231	ASN
1	C	232	THR
1	C	235	THR
1	C	237	ARG
1	C	242	THR
1	C	254	GLU
1	C	266	ILE
1	C	304	LEU
1	C	308	THR
1	C	316	LYS
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	435	GLN
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	615	VAL
1	C	619	LYS

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Mol	Chain	Res	Type
1	C	626	SER
1	C	635	SER
1	C	636	LEU
1	C	640	ASP
1	C	658	LEU
1	C	666	CYS
1	C	670	ILE
1	C	674	VAL
1	C	691	ILE
1	C	703	VAL
1	C	704	GLN
1	C	717	ARG
1	C	747	PHE
1	C	748	TYR
1	C	752	GLN
1	C	789	LYS
1	C	791	ARG
1	C	792	ILE
1	C	832	LEU
1	C	839	LEU
1	C	866	ILE
1	C	880	GLU
1	C	881	LEU
1	C	969	LEU
1	C	978	GLU
1	C	1027	GLN
1	C	1047	ILE
1	C	1057	ARG
1	C	1086	THR
1	C	1093	ARG
1	C	1110	ILE
1	C	1117	THR
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	1316	THR

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Mol	Chain	Res	Type
1	D	8	ASP
1	D	20	THR
1	D	28	VAL
1	D	43	THR
1	D	44	LYS
1	D	45	TYR
1	D	59	ILE
1	D	66	SER
1	D	97	SER
1	D	115	THR
1	D	117	CYS
1	D	120	CYS
1	D	127	SER
1	D	132	LEU
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	299	ASN
1	D	304	LEU
1	D	308	THR
1	D	316	LYS
1	D	338	LEU
1	D	344	LEU
1	D	362	ARG
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	435	GLN
1	D	470	VAL

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Mol	Chain	Res	Type
1	D	512	GLU
1	D	523	LEU
1	D	531	LEU
1	D	549	LEU
1	D	569	ASP
1	D	605	VAL
1	D	615	VAL
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	703	VAL
1	D	717	ARG
1	D	747	PHE
1	D	748	TYR
1	D	752	GLN
1	D	789	LYS
1	D	791	ARG
1	D	792	ILE
1	D	832	LEU
1	D	839	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	1110	ILE
1	D	1117	THR
1	D	1154	ILE
1	D	1224	LEU
1	D	1230	HIS
1	D	1240	ILE
1	D	1247	SER

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Mol	Chain	Res	Type
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 (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	A	317	ASN
1	A	369	ASN
1	A	574	GLN
1	A	704	GLN
1	A	733	GLN
1	A	857	ASN
1	A	1067	HIS
1	A	1097	ASN
1	A	1100	GLN
1	B	113	HIS
1	B	208	GLN
1	B	317	ASN
1	B	369	ASN
1	B	388	GLN
1	B	694	GLN
1	B	704	GLN
1	B	733	GLN
1	B	984	ASN
1	B	1067	HIS
1	B	1097	ASN
1	B	1100	GLN
1	C	208	GLN
1	C	317	ASN
1	C	369	ASN
1	C	376	ASN
1	C	380	ASN
1	C	704	GLN
1	C	867	GLN
1	C	1067	HIS
1	C	1097	ASN
1	C	1100	GLN
1	D	208	GLN
1	D	317	ASN
1	D	551	HIS

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Mol	Chain	Res	Type
1	D	708	GLN
1	D	1097	ASN
1	D	1100	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
3	FES	A	3001	1	0,4,4	-	-	-		
3	FES	A	3002	1	0,4,4	-	-	-		
6	FAD	A	3005	-	53,58,58	1.26	6 (11%)	68,89,89	1.31	10 (14%)
6	FAD	B	3005	-	53,58,58	1.27	5 (9%)	68,89,89	1.50	14 (20%)
3	FES	D	3002	1	0,4,4	-	-	-		
6	FAD	D	3005	-	53,58,58	1.27	5 (9%)	68,89,89	1.30	10 (14%)
5	MOS	A	3004	4	0,3,3	-	-	-		
4	MTE	B	3003	5	21,26,26	1.35	2 (9%)	21,40,40	2.15	8 (38%)
5	MOS	B	3004	4	0,3,3	-	-	-		
5	MOS	D	3004	4	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	MOS	C	3004	4	0,3,3	-	-	-		
3	FES	B	3002	1	0,4,4	-	-	-		
3	FES	D	3001	1	0,4,4	-	-	-		
4	MTE	C	3003	5	21,26,26	1.43	2 (9%)	21,40,40	2.54	7 (33%)
6	FAD	C	3005	-	53,58,58	1.27	6 (11%)	68,89,89	1.29	10 (14%)
3	FES	C	3001	1	0,4,4	-	-	-		
3	FES	B	3001	1	0,4,4	-	-	-		
3	FES	C	3002	1	0,4,4	-	-	-		
4	MTE	D	3003	5	21,26,26	1.37	2 (9%)	21,40,40	2.17	6 (28%)
4	MTE	A	3003	5	21,26,26	1.30	2 (9%)	21,40,40	2.18	7 (33%)

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	C	3001	1	-	-	0/1/1/1
3	FES	B	3001	1	-	-	0/1/1/1
3	FES	A	3001	1	-	-	0/1/1/1
3	FES	A	3002	1	-	-	0/1/1/1
6	FAD	A	3005	-	-	8/30/50/50	0/6/6/6
4	MTE	B	3003	5	-	2/6/34/34	0/3/3/3
3	FES	C	3002	1	-	-	0/1/1/1
4	MTE	D	3003	5	-	4/6/34/34	0/3/3/3
6	FAD	B	3005	-	-	16/30/50/50	0/6/6/6
3	FES	B	3002	1	-	-	0/1/1/1
4	MTE	A	3003	5	-	0/6/34/34	0/3/3/3
4	MTE	C	3003	5	-	0/6/34/34	0/3/3/3
6	FAD	C	3005	-	-	17/30/50/50	0/6/6/6
3	FES	D	3001	1	-	-	0/1/1/1
3	FES	D	3002	1	-	-	0/1/1/1
6	FAD	D	3005	-	-	12/30/50/50	0/6/6/6

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3005	FAD	C9A-C5X	5.13	1.49	1.41
6	C	3005	FAD	C9A-C5X	5.08	1.49	1.41
6	D	3005	FAD	C9A-C5X	4.88	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	3005	FAD	C9A-C5X	4.86	1.49	1.41
4	C	3003	MTE	C9-C4	4.68	1.47	1.41
4	D	3003	MTE	C9-C4	4.48	1.47	1.41
4	B	3003	MTE	C9-C4	4.20	1.47	1.41
4	A	3003	MTE	C9-C4	4.05	1.47	1.41
4	B	3003	MTE	C9-C10	3.61	1.48	1.41
4	C	3003	MTE	C9-C10	3.30	1.47	1.41
6	B	3005	FAD	C8-C7	3.29	1.49	1.40
4	A	3003	MTE	C9-C10	3.27	1.47	1.41
6	D	3005	FAD	C8-C7	3.23	1.49	1.40
4	D	3003	MTE	C9-C10	3.21	1.47	1.41
6	C	3005	FAD	C8-C7	3.19	1.48	1.40
6	A	3005	FAD	C8-C7	3.11	1.48	1.40
6	D	3005	FAD	C4-N3	-2.90	1.33	1.38
6	A	3005	FAD	C4-N3	-2.75	1.33	1.38
6	B	3005	FAD	C4-N3	-2.75	1.33	1.38
6	C	3005	FAD	C4-N3	-2.65	1.33	1.38
6	D	3005	FAD	C5X-N5	-2.34	1.34	1.39
6	A	3005	FAD	C5A-C4A	2.30	1.47	1.40
6	C	3005	FAD	C5A-C4A	2.29	1.47	1.40
6	C	3005	FAD	C5X-N5	-2.29	1.35	1.39
6	A	3005	FAD	C5X-N5	-2.28	1.35	1.39
6	B	3005	FAD	C5X-N5	-2.27	1.35	1.39
6	B	3005	FAD	C5A-C4A	2.23	1.46	1.40
6	D	3005	FAD	C5A-C4A	2.20	1.46	1.40
6	C	3005	FAD	C4X-N5	2.08	1.34	1.30
6	A	3005	FAD	C4X-N5	2.07	1.34	1.30

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	3003	MTE	O3'-C7-C6	-7.24	104.14	108.96
6	B	3005	FAD	C1'-N10-C9A	5.51	129.70	120.51
4	B	3003	MTE	O3'-C7-C6	-4.32	106.08	108.96
4	D	3003	MTE	C10-N8-C7	-4.30	115.24	123.67
4	C	3003	MTE	C4-C9-N5	4.23	122.67	119.12
4	A	3003	MTE	C4-C9-N5	4.11	122.57	119.12
4	D	3003	MTE	C4-C9-N5	3.94	122.43	119.12
4	A	3003	MTE	O3'-C7-N8	3.75	112.42	108.57
4	A	3003	MTE	C2-N3-C4	3.75	121.88	115.93
4	D	3003	MTE	C2-N3-C4	3.68	121.78	115.93
4	A	3003	MTE	C10-N8-C7	-3.67	116.48	123.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	3003	MTE	O3'-C7-C6	-3.66	106.52	108.96
4	C	3003	MTE	C2-N3-C4	3.65	121.72	115.93
4	C	3003	MTE	C10-N8-C7	-3.60	116.61	123.67
6	A	3005	FAD	P-O3P-PA	-3.57	120.58	132.83
6	B	3005	FAD	N3A-C2A-N1A	-3.47	123.25	128.68
4	B	3003	MTE	C2-N3-C4	3.30	121.17	115.93
6	D	3005	FAD	N3A-C2A-N1A	-3.26	123.59	128.68
6	B	3005	FAD	C4X-C10-N10	3.19	121.14	116.48
4	B	3003	MTE	C10-N8-C7	-3.17	117.47	123.67
6	C	3005	FAD	N3A-C2A-N1A	-3.15	123.76	128.68
4	B	3003	MTE	C10-C9-C4	3.09	117.31	114.57
6	A	3005	FAD	N3A-C2A-N1A	-3.05	123.91	128.68
4	D	3003	MTE	C2-N1-C10	2.99	121.24	114.54
4	B	3003	MTE	C2-N1-C10	2.98	121.22	114.54
4	B	3003	MTE	C4-C9-N5	2.92	121.57	119.12
6	D	3005	FAD	P-O3P-PA	-2.86	123.02	132.83
6	B	3005	FAD	C4-C4X-N5	2.85	122.29	118.23
6	D	3005	FAD	C4X-C10-N1	-2.84	118.14	124.73
6	A	3005	FAD	C4X-C10-N1	-2.82	118.18	124.73
6	A	3005	FAD	C4A-C5A-N7A	-2.82	106.46	109.40
6	C	3005	FAD	C4A-C5A-N7A	-2.81	106.47	109.40
4	C	3003	MTE	C2-N1-C10	2.79	120.80	114.54
4	A	3003	MTE	C2-N1-C10	2.77	120.75	114.54
4	A	3003	MTE	O3'-C7-C6	-2.77	107.12	108.96
6	C	3005	FAD	P-O3P-PA	-2.77	123.32	132.83
4	C	3003	MTE	C10-C9-C4	2.69	116.96	114.57
6	B	3005	FAD	P-O3P-PA	-2.62	123.83	132.83
6	D	3005	FAD	C4A-C5A-N7A	-2.61	106.68	109.40
6	C	3005	FAD	C4X-C10-N1	-2.60	118.71	124.73
6	A	3005	FAD	C3B-C2B-C1B	2.58	104.86	100.98
6	C	3005	FAD	C4-C4X-N5	2.57	121.89	118.23
6	D	3005	FAD	C3B-C2B-C1B	2.56	104.83	100.98
6	B	3005	FAD	C4X-C10-N1	-2.54	118.83	124.73
4	B	3003	MTE	O3'-C7-N8	2.48	111.11	108.57
6	C	3005	FAD	C4X-C10-N10	2.46	120.07	116.48
6	C	3005	FAD	O4-C4-C4X	-2.43	120.17	126.60
6	B	3005	FAD	C4A-C5A-N7A	-2.43	106.87	109.40
6	A	3005	FAD	C4-C4X-N5	2.42	121.67	118.23
6	D	3005	FAD	C4-C4X-N5	2.41	121.67	118.23
6	A	3005	FAD	C4X-C10-N10	2.38	119.95	116.48
4	D	3003	MTE	C10-C9-C4	2.36	116.66	114.57
6	B	3005	FAD	O4-C4-C4X	-2.33	120.42	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	3005	FAD	O4-C4-C4X	-2.27	120.58	126.60
4	C	3003	MTE	O2P-P-O4'	-2.26	100.71	106.73
6	A	3005	FAD	C10-N1-C2	2.26	121.42	116.90
6	B	3005	FAD	C9A-N10-C10	-2.24	117.28	120.77
6	A	3005	FAD	O4-C4-C4X	-2.23	120.68	126.60
6	B	3005	FAD	O2-C2-N1	-2.21	118.16	121.83
6	D	3005	FAD	C10-N1-C2	2.21	121.32	116.90
6	D	3005	FAD	C4X-C10-N10	2.19	119.67	116.48
6	B	3005	FAD	C10-N1-C2	2.18	121.26	116.90
6	C	3005	FAD	C10-N1-C2	2.18	121.25	116.90
6	B	3005	FAD	C3B-C2B-C1B	2.14	104.20	100.98
6	C	3005	FAD	O2-C2-N1	-2.13	118.30	121.83
4	A	3003	MTE	C10-C9-C4	2.13	116.46	114.57
4	B	3003	MTE	O3P-P-O2P	2.10	115.65	107.64
6	D	3005	FAD	C4X-C4-N3	2.07	118.45	113.19
6	B	3005	FAD	C4X-C4-N3	2.06	118.43	113.19
6	C	3005	FAD	C4X-C4-N3	2.05	118.40	113.19
6	A	3005	FAD	C4X-C4-N3	2.04	118.37	113.19
6	B	3005	FAD	C5'-C4'-C3'	-2.01	108.32	112.20

There are no chirality outliers.

All (59) 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
4	D	3003	MTE	C4'-O4'-P-O3P
6	A	3005	FAD	C5B-O5B-PA-O2A
6	A	3005	FAD	C5B-O5B-PA-O3P
6	B	3005	FAD	C5B-O5B-PA-O1A
6	B	3005	FAD	C5B-O5B-PA-O2A
6	B	3005	FAD	C3B-C4B-C5B-O5B
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	C	3005	FAD	C5B-O5B-PA-O1A
6	C	3005	FAD	C5B-O5B-PA-O3P
6	C	3005	FAD	C2'-C1'-N10-C9A

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

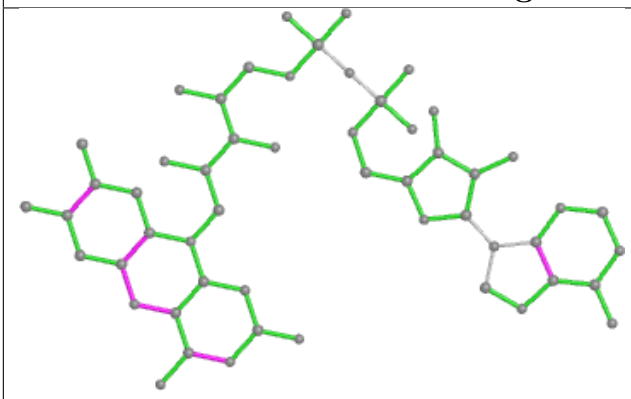
There are no ring outliers.

16 monomers are involved in 82 short contacts:

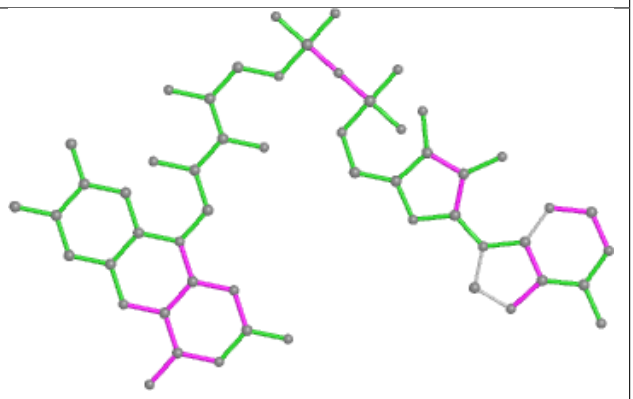
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3002	FES	1	0
6	A	3005	FAD	8	0
6	B	3005	FAD	14	0
3	D	3002	FES	2	0
6	D	3005	FAD	15	0
5	A	3004	MOS	2	0
4	B	3003	MTE	1	0
5	B	3004	MOS	2	0
5	D	3004	MOS	2	0
5	C	3004	MOS	2	0
3	B	3002	FES	1	0
4	C	3003	MTE	3	0
6	C	3005	FAD	21	0
3	C	3002	FES	1	0
4	D	3003	MTE	3	0
4	A	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

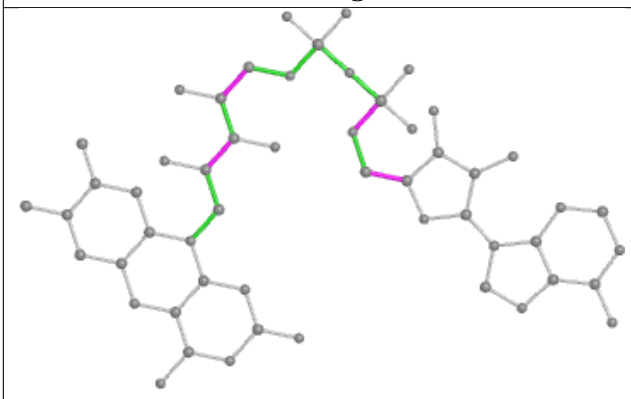
Ligand FAD A 3005



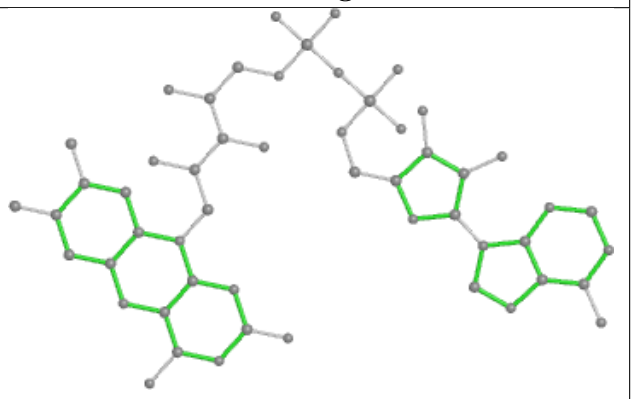
Bond lengths



Bond angles

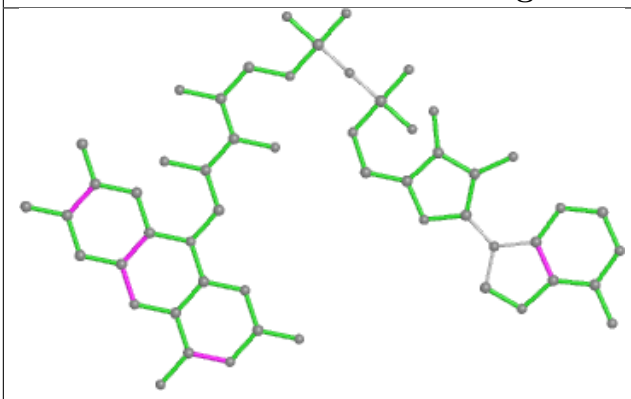


Torsions



Rings

Ligand FAD B 3005



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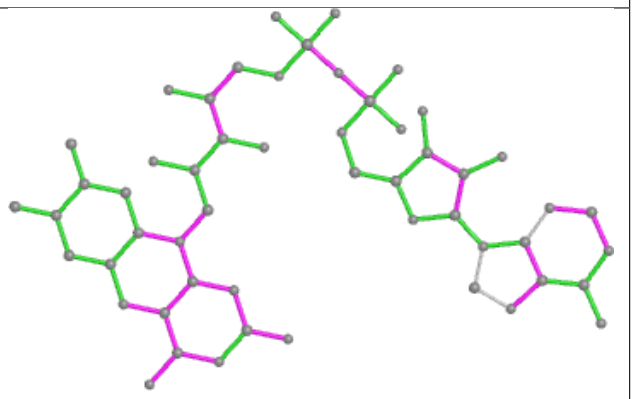

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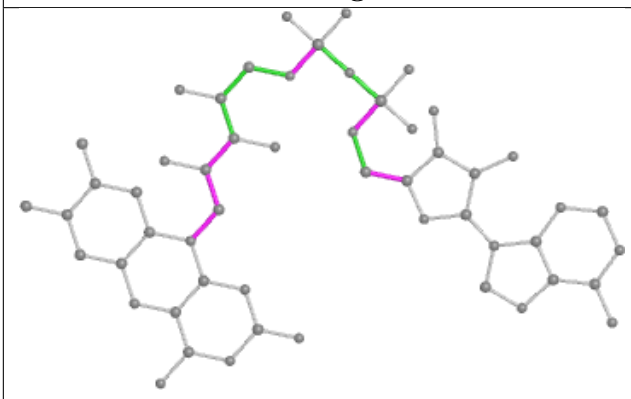

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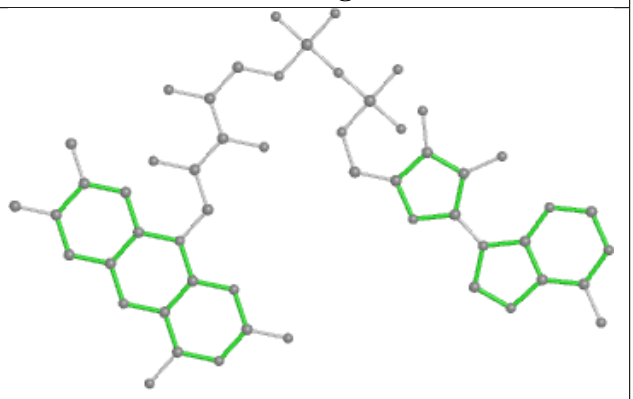
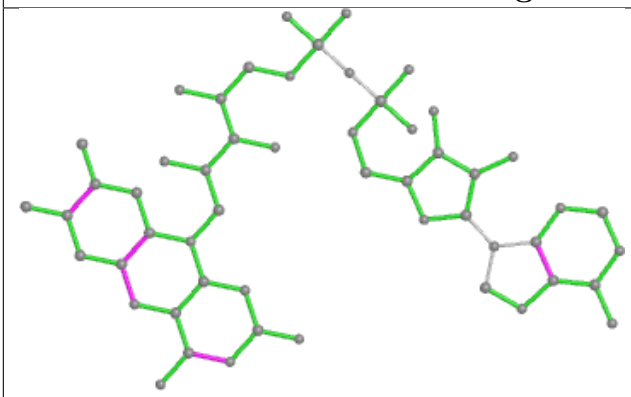


Rings

Ligand FAD D 3005



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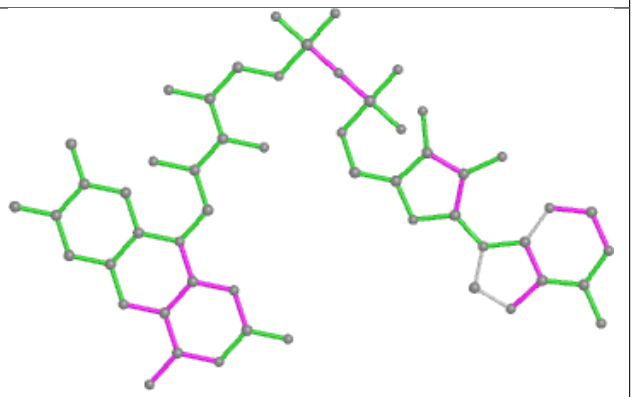

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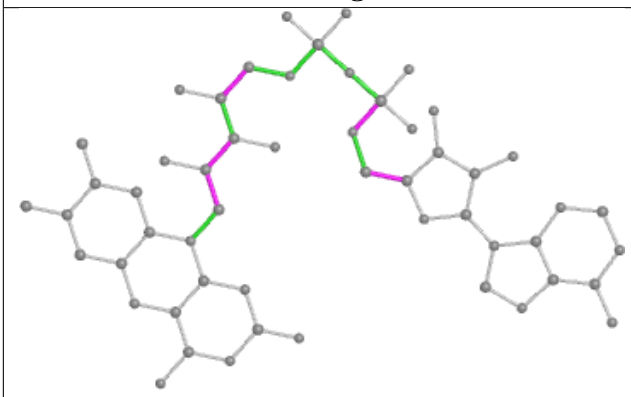
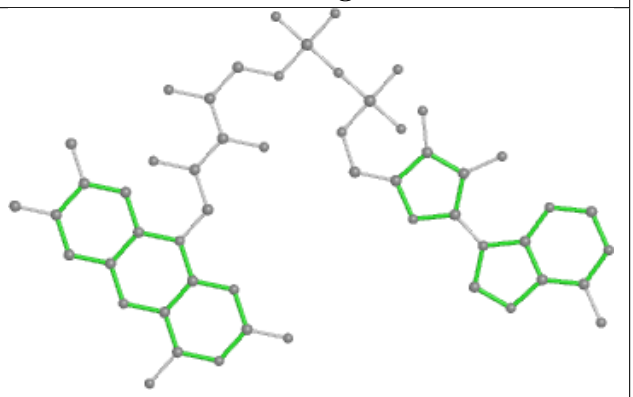
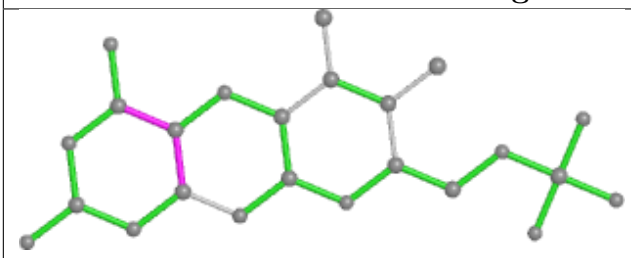


Torsions



Rings

Ligand MTE B 3003



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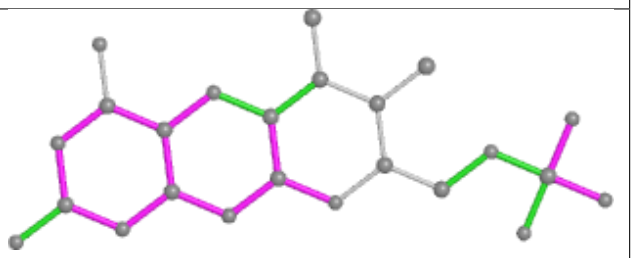
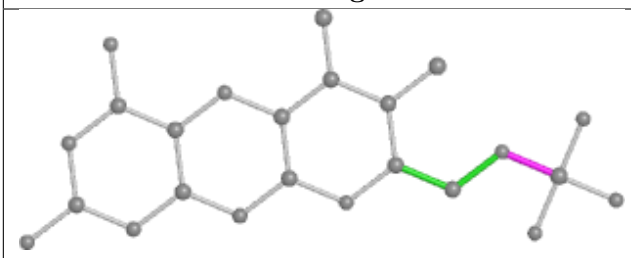
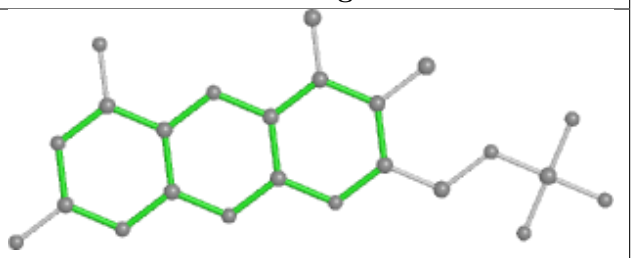


Bond angles

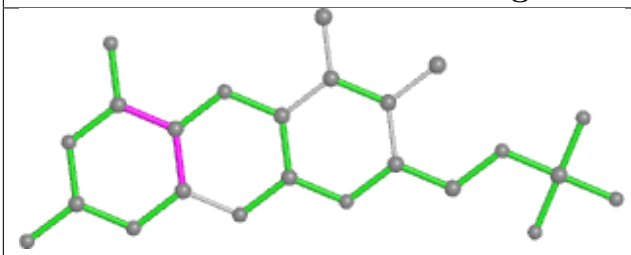


Torsions



Rings

Ligand MTE C 3003



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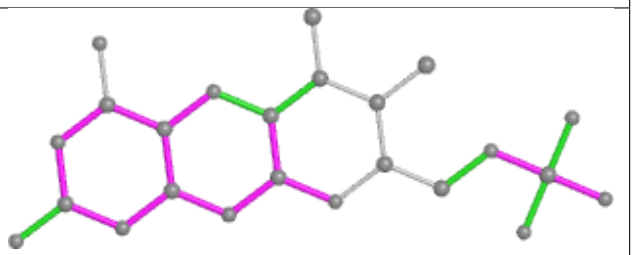

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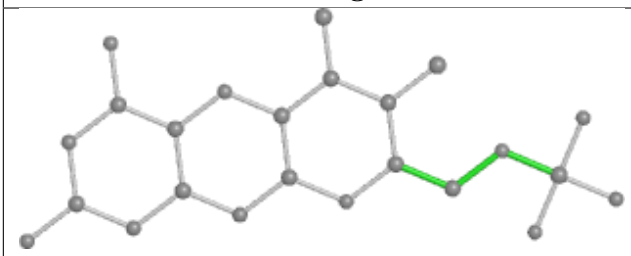

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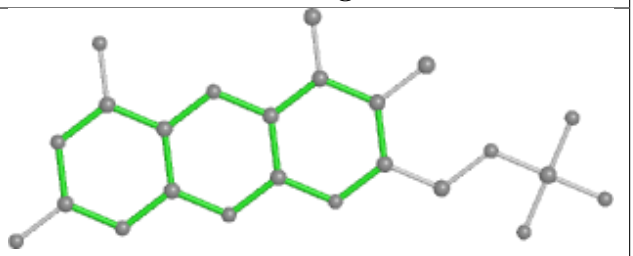
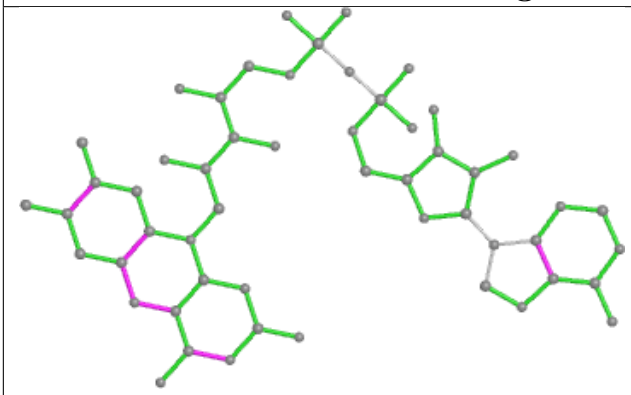


Rings

Ligand FAD C 3005



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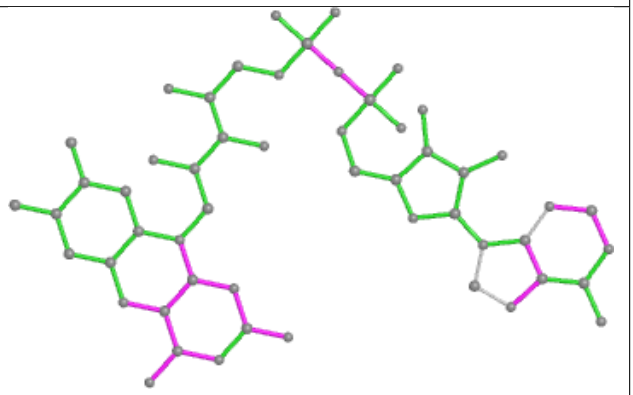

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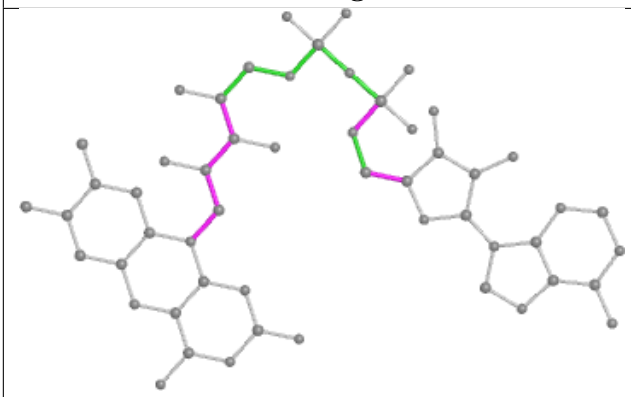

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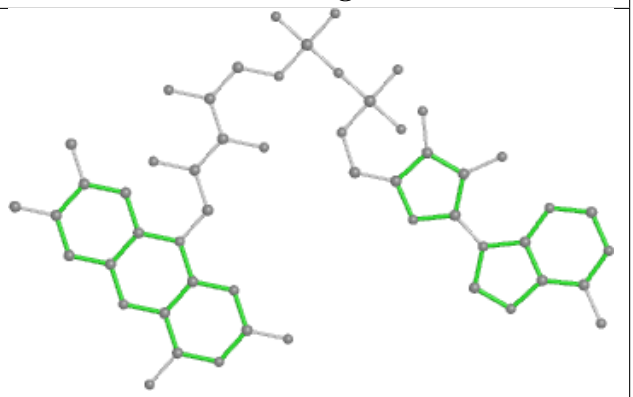
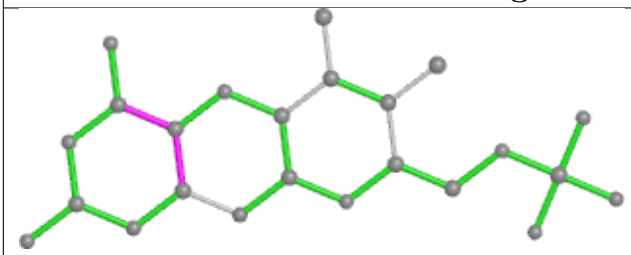


Rings

Ligand MTE D 3003



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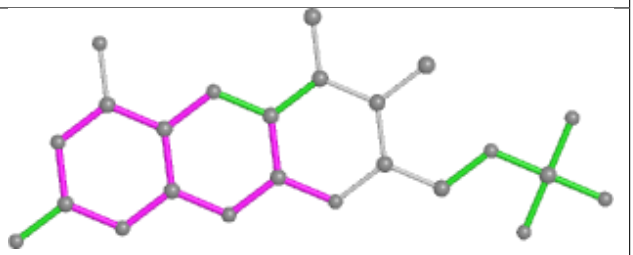

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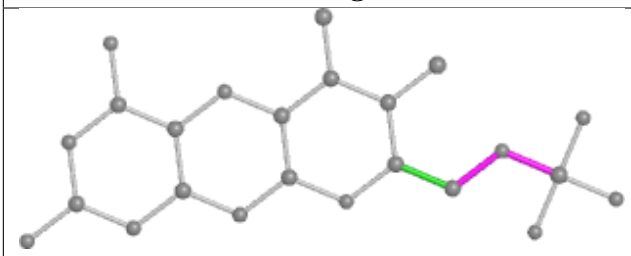

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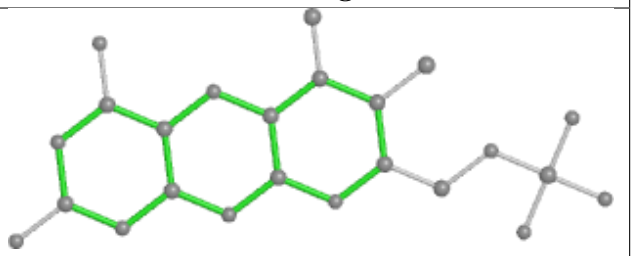
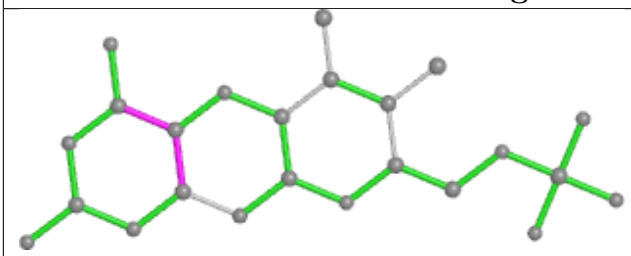


Rings

Ligand MTE A 3003



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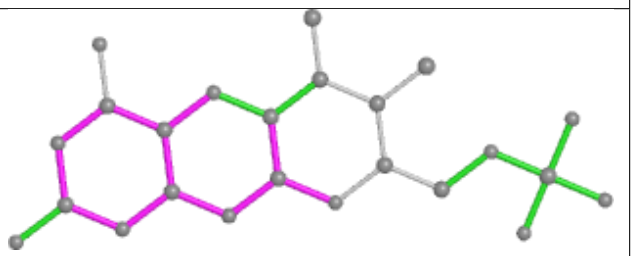

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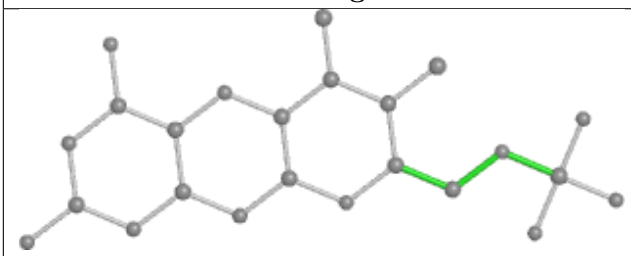
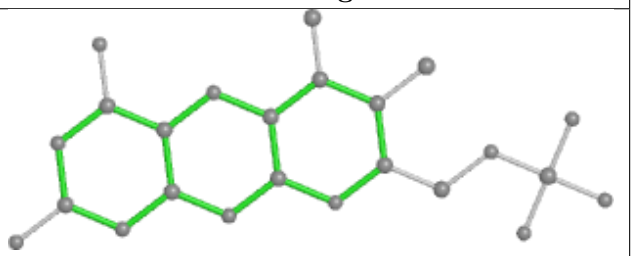


Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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(Å^2)	Q<0.9
1	A	1253/1335 (93%)	0.43	69 (5%)	25	30	12, 40, 70, 88	0
1	B	1262/1335 (94%)	0.44	68 (5%)	25	30	10, 39, 67, 87	0
1	C	1244/1335 (93%)	0.48	88 (7%)	16	19	18, 43, 73, 99	0
1	D	1257/1335 (94%)	0.66	125 (9%)	7	9	20, 45, 79, 97	0
All	All	5016/5340 (93%)	0.50	350 (6%)	16	19	10, 42, 73, 99	0

All (350) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	477	CYS	7.0
1	C	937	ALA	6.1
1	D	492	ASP	5.3
1	B	728	PHE	5.1
1	D	278	THR	5.0
1	B	403	ALA	5.0
1	C	859	GLY	5.0
1	D	494	GLY	5.0
1	D	548	LYS	5.0
1	C	497	ILE	4.9
1	D	456	ILE	4.7
1	C	473	ALA	4.7
1	D	545	ILE	4.7
1	C	303	GLY	4.7
1	D	421	LYS	4.6
1	D	480	LEU	4.6
1	A	545	ILE	4.6
1	A	484	CYS	4.5
1	C	731	ALA	4.5
1	C	730	CYS	4.5
1	D	482	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	506	ALA	4.3
1	A	303	GLY	4.3
1	A	424	PHE	4.2
1	C	454	ASN	4.1
1	D	549	LEU	4.1
1	C	420	SER	4.1
1	C	458	ASP	4.1
1	C	424	PHE	4.1
1	B	727	ALA	4.0
1	A	490	LEU	4.0
1	C	484	CYS	4.0
1	A	327	PRO	4.0
1	A	417	PRO	4.0
1	B	477	CYS	3.9
1	D	458	ASP	3.8
1	C	373	GLY	3.8
1	C	995	GLN	3.8
1	D	727	ALA	3.8
1	D	572	PHE	3.8
1	A	216	LEU	3.7
1	C	480	LEU	3.7
1	B	896	ILE	3.7
1	A	997	PHE	3.6
1	B	527	TYR	3.6
1	D	1234	ILE	3.6
1	D	424	PHE	3.6
1	D	484	CYS	3.6
1	D	457	THR	3.5
1	D	726	GLU	3.5
1	B	857	ASN	3.5
1	D	277	PHE	3.5
1	D	304	LEU	3.4
1	D	461	ILE	3.4
1	B	373	GLY	3.4
1	D	447	VAL	3.4
1	D	323	VAL	3.4
1	B	549	LEU	3.4
1	D	536	THR	3.4
1	C	722	GLY	3.4
1	B	572	PHE	3.4
1	A	448	VAL	3.4
1	C	729	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	481	ILE	3.3
1	C	1285	ALA	3.3
1	A	553	LEU	3.3
1	D	524	PHE	3.3
1	D	1295	ILE	3.3
1	D	730	CYS	3.3
1	A	420	SER	3.3
1	B	1115	SER	3.3
1	B	1249	LEU	3.2
1	A	326	LEU	3.2
1	D	728	PHE	3.2
1	C	933	SER	3.2
1	D	734	ILE	3.2
1	A	296	VAL	3.2
1	D	624	ILE	3.2
1	D	857	ASN	3.2
1	B	7	SER	3.2
1	C	524	PHE	3.1
1	C	447	VAL	3.1
1	B	496	MET	3.1
1	D	899	LEU	3.1
1	A	399	GLY	3.1
1	D	419	SER	3.1
1	C	534	LEU	3.1
1	D	398	ALA	3.1
1	D	377	CYS	3.1
1	B	398	ALA	3.1
1	C	477	CYS	3.0
1	D	274	HIS	3.0
1	C	483	ARG	3.0
1	D	449	PHE	3.0
1	D	448	VAL	3.0
1	A	466	ILE	3.0
1	D	459	LEU	3.0
1	C	858	ASN	3.0
1	C	701	VAL	3.0
1	D	625	ILE	3.0
1	D	1109	ILE	3.0
1	B	504	LEU	3.0
1	C	499	GLU	2.9
1	D	737	GLY	2.9
1	A	475	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1320	PRO	2.9
1	A	1285	ALA	2.9
1	B	730	CYS	2.9
1	A	527	TYR	2.9
1	D	487	GLU	2.9
1	D	445	MET	2.9
1	D	327	PRO	2.9
1	A	998	TRP	2.9
1	A	938	LYS	2.8
1	D	1318	LEU	2.8
1	B	422	TRP	2.8
1	B	699	MET	2.8
1	D	1150	GLY	2.8
1	C	570	VAL	2.8
1	A	734	ILE	2.8
1	C	481	ILE	2.8
1	C	1290	ARG	2.8
1	D	454	ASN	2.8
1	D	281	SER	2.8
1	A	709	TYR	2.8
1	D	455	THR	2.8
1	D	665	ILE	2.8
1	C	572	PHE	2.8
1	B	1209	GLY	2.8
1	A	376	ASN	2.7
1	C	216	LEU	2.7
1	B	734	ILE	2.7
1	A	492	ASP	2.7
1	C	856	MET	2.7
1	A	537	ARG	2.7
1	A	937	ALA	2.7
1	C	455	THR	2.7
1	D	729	GLN	2.7
1	C	527	TYR	2.7
1	C	978	GLU	2.7
1	A	523	LEU	2.7
1	D	576	LEU	2.7
1	B	858	ASN	2.7
1	C	275	MET	2.7
1	A	1290	ARG	2.7
1	D	981	SER	2.6
1	D	452	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	699	MET	2.6
1	C	1115	SER	2.6
1	D	497	ILE	2.6
1	D	575	PRO	2.6
1	D	708	GLN	2.6
1	D	715	PRO	2.6
1	B	233	VAL	2.6
1	C	422	TRP	2.6
1	B	1230	HIS	2.6
1	C	857	ASN	2.6
1	D	714	GLY	2.6
1	D	803	PHE	2.6
1	B	323	VAL	2.6
1	D	1114	PRO	2.6
1	A	906	CYS	2.6
1	A	480	LEU	2.6
1	C	1148	GLU	2.6
1	D	322	VAL	2.5
1	B	1114	PRO	2.5
1	B	338	LEU	2.5
1	A	991	GLU	2.5
1	C	491	ASP	2.5
1	A	495	LYS	2.5
1	B	729	GLN	2.5
1	D	493	ALA	2.5
1	D	709	TYR	2.5
1	B	421	LYS	2.5
1	B	576	LEU	2.5
1	D	1205	VAL	2.5
1	D	526	PHE	2.5
1	D	335	CYS	2.5
1	B	459	LEU	2.5
1	D	531	LEU	2.5
1	C	532	LYS	2.5
1	B	988	ALA	2.5
1	C	498	CYS	2.5
1	C	490	LEU	2.5
1	D	395	HIS	2.5
1	B	419	SER	2.5
1	A	992	PHE	2.5
1	A	217	ILE	2.4
1	C	725	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	804	GLY	2.4
1	C	536	THR	2.4
1	A	334	TYR	2.4
1	D	987	LYS	2.4
1	D	1113	ASN	2.4
1	B	1252	THR	2.4
1	D	1250	THR	2.4
1	A	280	VAL	2.4
1	C	530	VAL	2.4
1	B	1228	GLY	2.4
1	C	459	LEU	2.4
1	D	570	VAL	2.4
1	A	547	GLN	2.4
1	C	302	GLN	2.4
1	D	748	TYR	2.4
1	D	743	GLY	2.4
1	D	1329	PRO	2.4
1	B	491	ASP	2.4
1	C	848	LEU	2.4
1	D	1043	LEU	2.4
1	C	479	GLN	2.4
1	B	856	MET	2.4
1	C	463	TYR	2.4
1	B	455	THR	2.4
1	B	485	TRP	2.4
1	B	478	ARG	2.4
1	C	7	SER	2.4
1	C	326	LEU	2.4
1	C	65	ILE	2.4
1	A	455	THR	2.4
1	A	1172	LEU	2.4
1	B	1210	LEU	2.4
1	D	842	GLY	2.3
1	A	447	VAL	2.3
1	A	1318	LEU	2.3
1	D	725	GLU	2.3
1	B	625	ILE	2.3
1	B	709	TYR	2.3
1	A	478	ARG	2.3
1	B	490	LEU	2.3
1	D	486	ASP	2.3
1	A	546	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	482	GLY	2.3
1	D	1112	GLN	2.3
1	A	169	PRO	2.3
1	B	545	ILE	2.3
1	C	537	ARG	2.3
1	D	858	ASN	2.3
1	D	934	ALA	2.3
1	D	1115	SER	2.3
1	A	331	THR	2.3
1	A	154	CYS	2.3
1	C	990	ASP	2.3
1	D	1253	PRO	2.3
1	B	1116	GLY	2.3
1	D	378	ILE	2.3
1	A	47	CYS	2.3
1	A	477	CYS	2.3
1	B	377	CYS	2.3
1	C	47	CYS	2.3
1	A	942	PRO	2.2
1	C	421	LYS	2.2
1	A	481	ILE	2.2
1	C	1318	LEU	2.2
1	B	694	GLN	2.2
1	C	708	GLN	2.2
1	C	456	ILE	2.2
1	B	536	THR	2.2
1	C	997	PHE	2.2
1	C	1252	THR	2.2
1	D	553	LEU	2.2
1	C	723	ASN	2.2
1	D	898	ASN	2.2
1	B	238	GLY	2.2
1	A	323	VAL	2.2
1	D	537	ARG	2.2
1	C	728	PHE	2.2
1	D	1189	PHE	2.2
1	A	994	GLN	2.2
1	D	533	GLN	2.2
1	D	422	TRP	2.2
1	C	495	LYS	2.2
1	D	478	ARG	2.2
1	D	498	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	424	PHE	2.2
1	B	726	GLU	2.2
1	B	169	PRO	2.2
1	D	735	LEU	2.2
1	B	869	TYR	2.2
1	A	1235	ALA	2.2
1	D	744	GLN	2.2
1	D	1203	ALA	2.2
1	A	520	ILE	2.2
1	C	417	PRO	2.2
1	D	47	CYS	2.2
1	D	722	GLY	2.2
1	B	537	ARG	2.2
1	D	420	SER	2.2
1	D	753	SER	2.2
1	D	869	TYR	2.2
1	D	532	LYS	2.2
1	C	468	ALA	2.2
1	D	863	ALA	2.2
1	D	915	ALA	2.2
1	B	497	ILE	2.2
1	D	1269	THR	2.2
1	A	494	GLY	2.2
1	B	1108	PRO	2.2
1	C	868	LEU	2.2
1	A	551	HIS	2.1
1	A	1321	GLN	2.1
1	D	479	GLN	2.1
1	C	496	MET	2.1
1	A	1150	GLY	2.1
1	B	456	ILE	2.1
1	C	494	GLY	2.1
1	C	509	GLY	2.1
1	B	557	PRO	2.1
1	C	568	GLN	2.1
1	D	547	GLN	2.1
1	A	1146	ASP	2.1
1	D	386	GLY	2.1
1	A	1251	PRO	2.1
1	C	1315	PHE	2.1
1	A	1209	GLY	2.1
1	A	989	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	552	ILE	2.1
1	B	744	GLN	2.1
1	B	489	MET	2.1
1	C	525	MET	2.1
1	D	280	VAL	2.1
1	B	484	CYS	2.1
1	B	707	LEU	2.1
1	B	636	LEU	2.1
1	D	1206	GLN	2.1
1	D	802	ALA	2.1
1	C	711	SER	2.1
1	C	916	PHE	2.1
1	D	919	PHE	2.1
1	C	547	GLN	2.1
1	C	854	GLY	2.1
1	B	330	LYS	2.1
1	D	475	LYS	2.1
1	D	1211	TYR	2.0
1	A	741	LEU	2.0
1	B	553	LEU	2.0
1	D	916	PHE	2.0
1	C	486	ASP	2.0
1	D	279	ASP	2.0
1	C	457	THR	2.0
1	A	419	SER	2.0
1	A	549	LEU	2.0
1	B	275	MET	2.0
1	C	1253	PRO	2.0
1	D	1148	GLU	2.0
1	A	533	GLN	2.0
1	C	994	GLN	2.0
1	D	152	CYS	2.0
1	D	1117	THR	2.0
1	C	983	TYR	2.0
1	D	1232	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

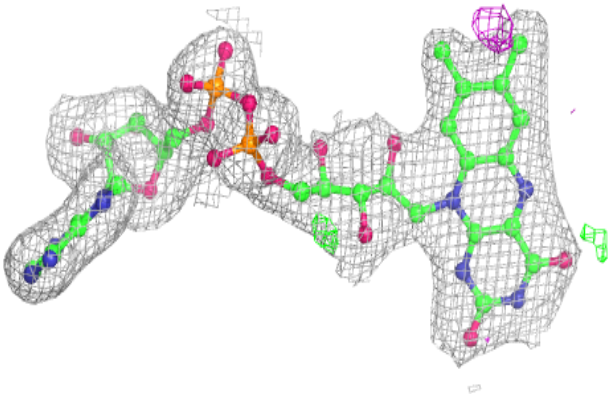
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

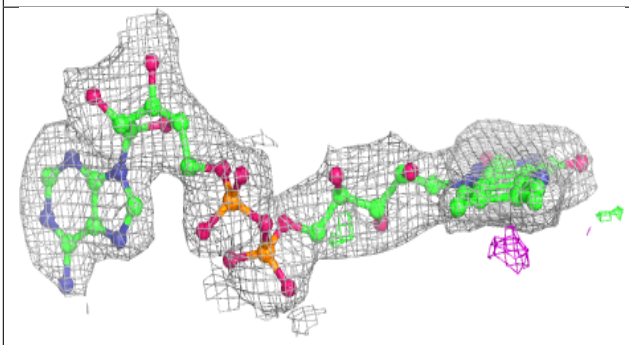
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	C	2337	1/1	0.89	0.16	50,50,50,50	0
2	NA	A	2337	1/1	0.90	0.14	26,26,26,26	0
6	FAD	B	3005	53/53	0.94	0.16	7,31,43,51	0
6	FAD	C	3005	53/53	0.94	0.15	9,31,49,50	0
6	FAD	D	3005	53/53	0.94	0.15	6,33,46,53	0
2	NA	B	2337	1/1	0.96	0.16	12,12,12,12	0
4	MTE	B	3003	24/24	0.96	0.17	15,35,49,67	0
6	FAD	A	3005	53/53	0.96	0.14	9,28,45,49	0
4	MTE	A	3003	24/24	0.97	0.17	12,27,37,42	0
3	FES	C	3002	4/4	0.97	0.08	29,33,36,38	0
4	MTE	C	3003	24/24	0.97	0.16	7,32,46,61	0
4	MTE	D	3003	24/24	0.97	0.18	13,33,49,53	0
5	MOS	B	3004	4/4	0.98	0.15	42,55,69,77	0
5	MOS	D	3004	4/4	0.98	0.16	42,55,69,77	0
3	FES	A	3002	4/4	0.98	0.09	16,23,33,38	0
3	FES	B	3002	4/4	0.98	0.11	20,21,34,38	0
3	FES	C	3001	4/4	0.98	0.12	24,24,31,39	0
2	NA	D	2337	1/1	0.98	0.17	17,17,17,17	0
5	MOS	C	3004	4/4	0.99	0.09	42,55,69,77	0
3	FES	A	3001	4/4	0.99	0.14	19,20,23,26	0
3	FES	D	3001	4/4	0.99	0.13	15,23,23,26	0
3	FES	D	3002	4/4	0.99	0.10	15,24,25,41	0
5	MOS	A	3004	4/4	0.99	0.12	42,55,69,77	0
3	FES	B	3001	4/4	0.99	0.14	7,20,22,26	0

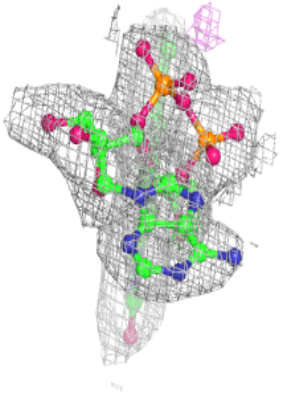
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

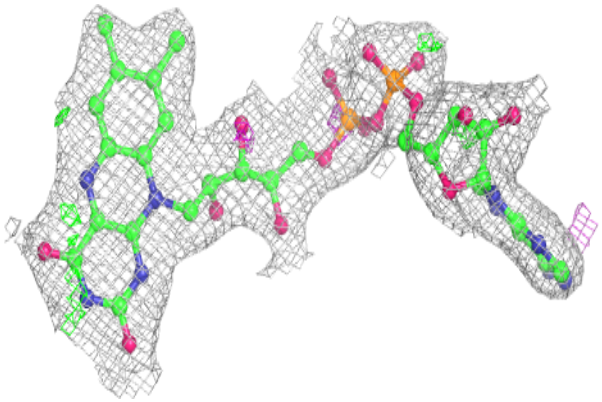


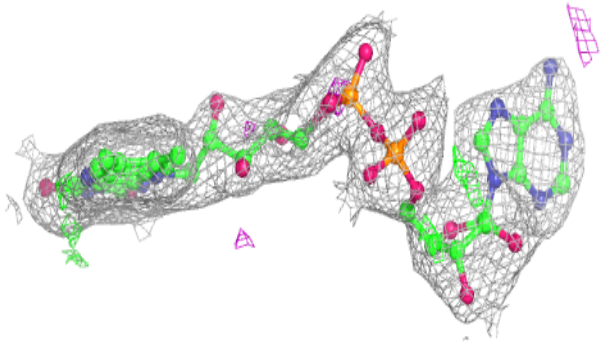


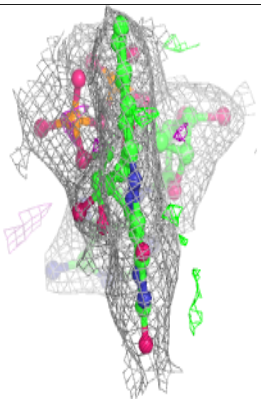


Electron density around FAD C 3005:

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

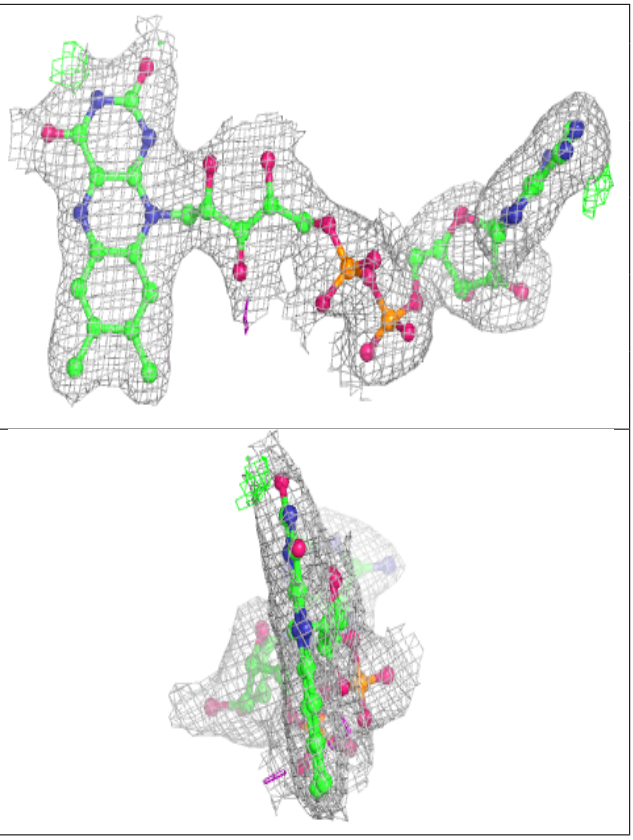


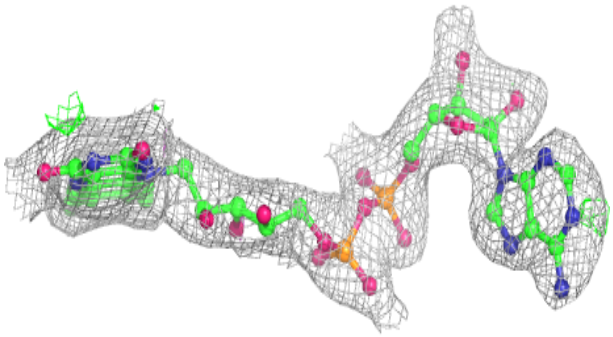




Electron density around FAD D 3005:

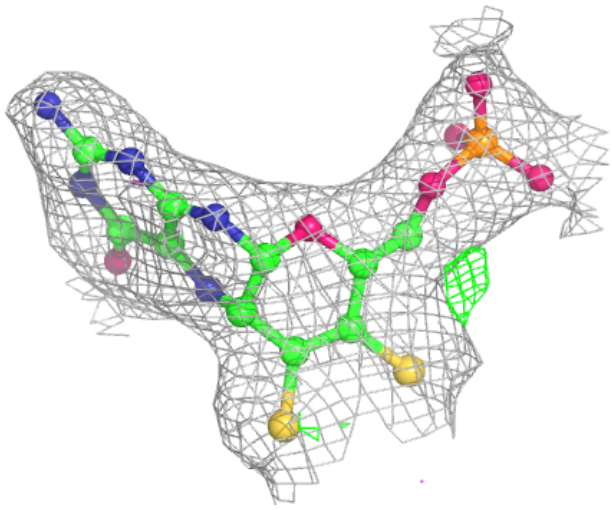
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

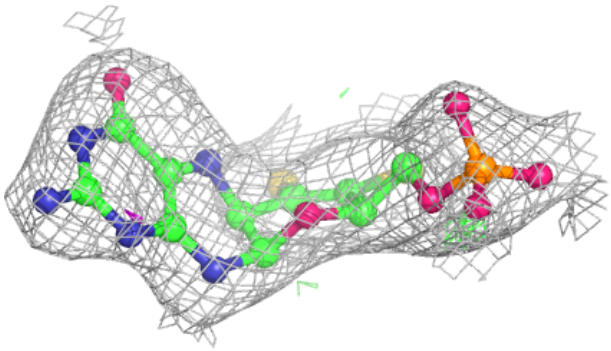


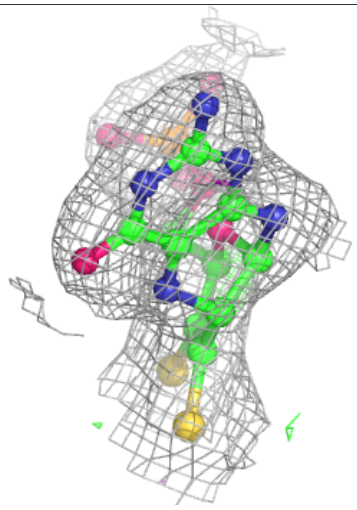


Electron density around MTE B 3003:

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

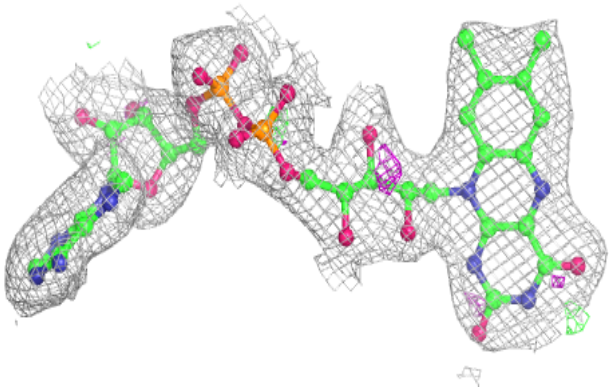


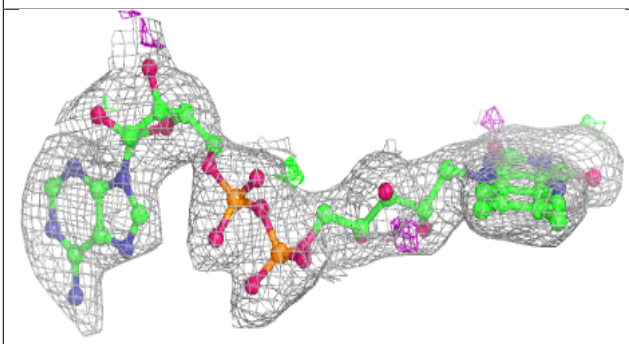


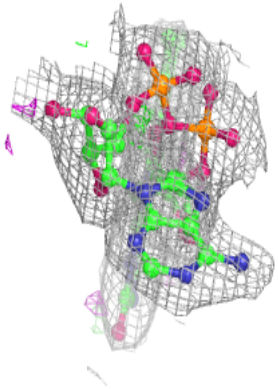


Electron density around FAD A 3005:

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

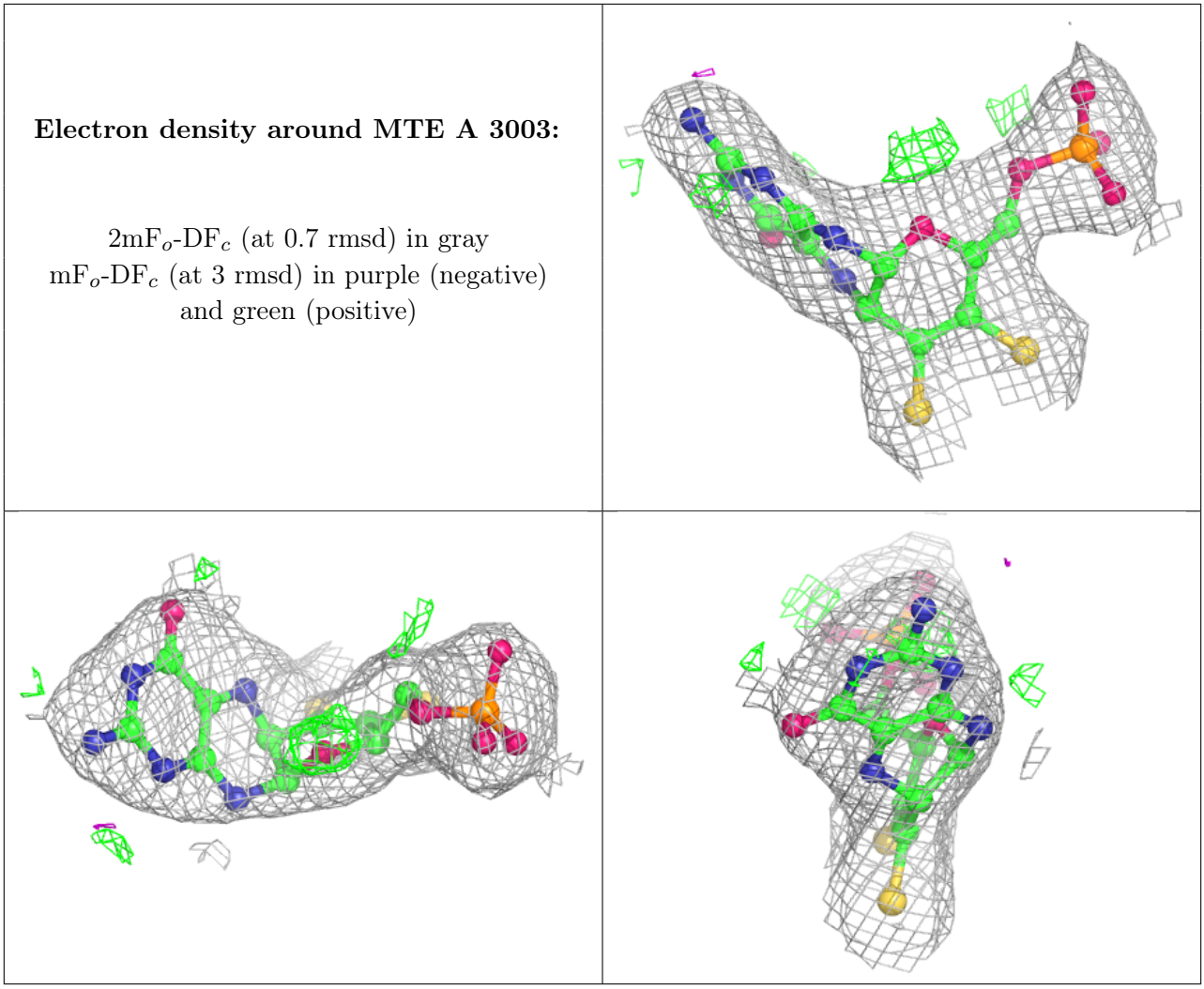






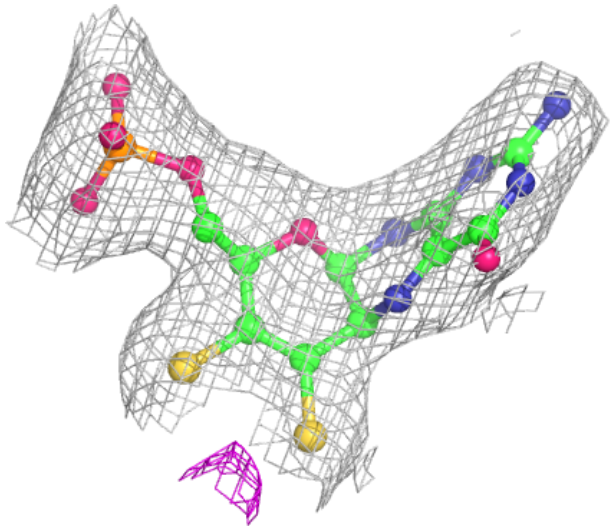
Electron density around MTE A 3003:

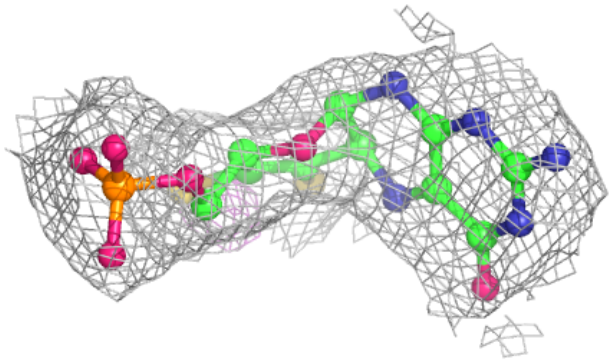
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

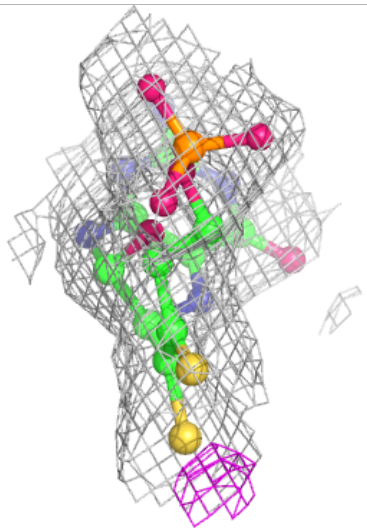


Electron density around MTE C 3003:

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

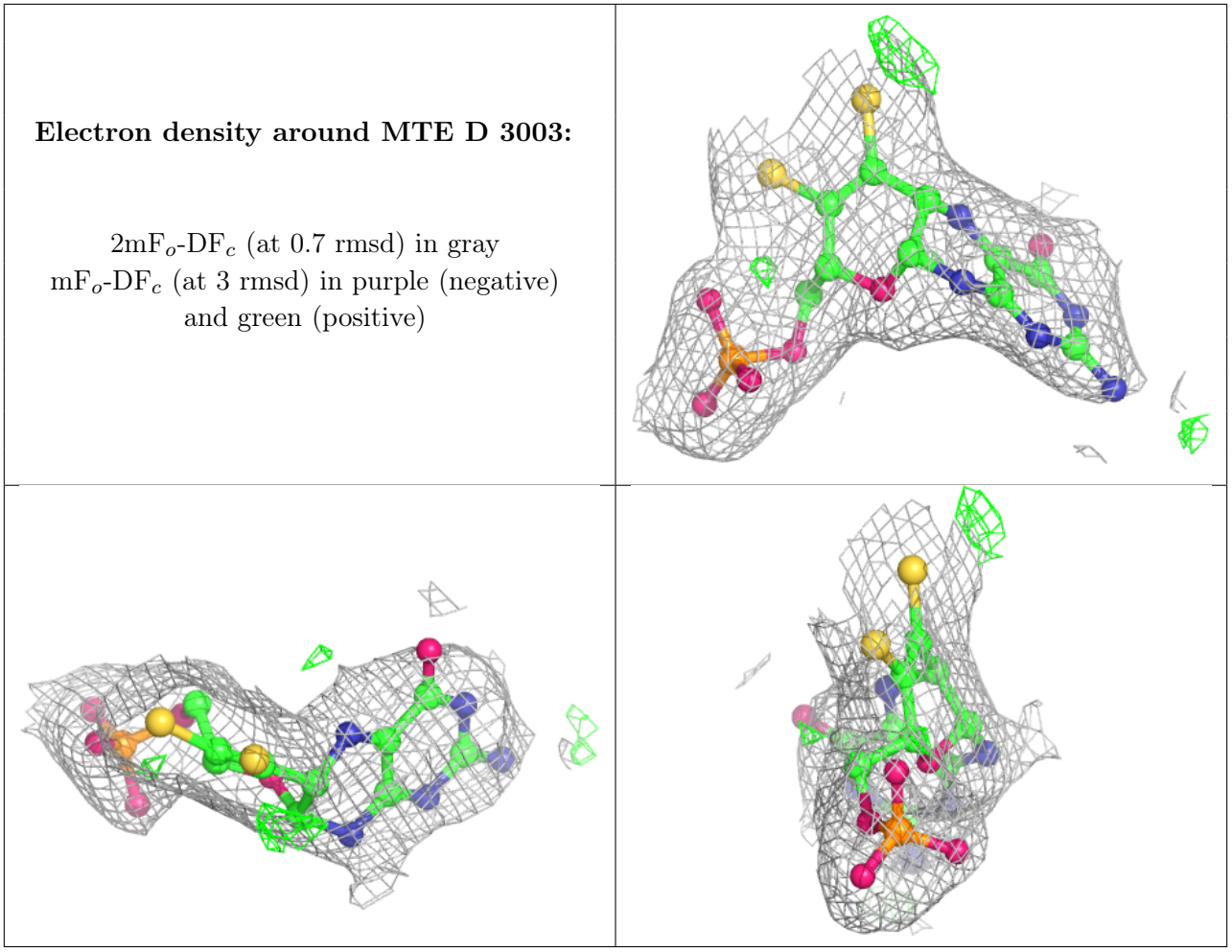






Electron density around MTE D 3003:

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



6.5 Other polymers

There are no such residues in this entry.