



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:56 am BST

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

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

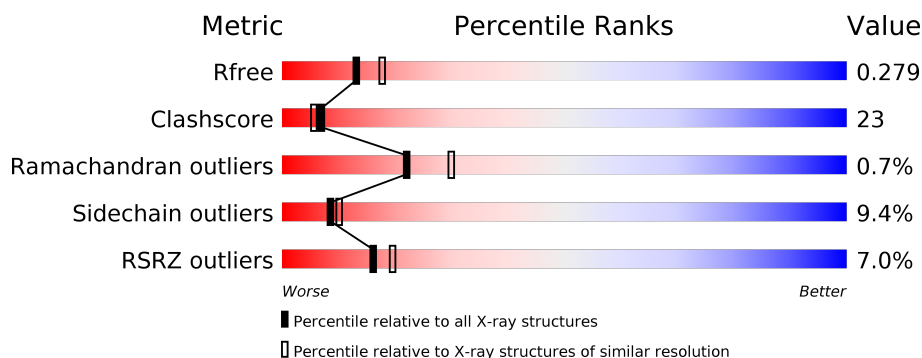
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1335	<div> <div>5%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>•</div> <div>6%</div> </div> </div>
1	B	1335	<div> <div>5%</div> <div> <div></div> <div>57%</div> <div>33%</div> <div>5%</div> <div>5%</div> </div> </div>
1	C	1335	<div> <div>7%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>•</div> <div>7%</div> </div> </div>
1	D	1335	<div> <div>9%</div> <div> <div></div> <div>58%</div> <div>32%</div> <div>•</div> <div>6%</div> </div> </div>

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 crite-

ria:

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).

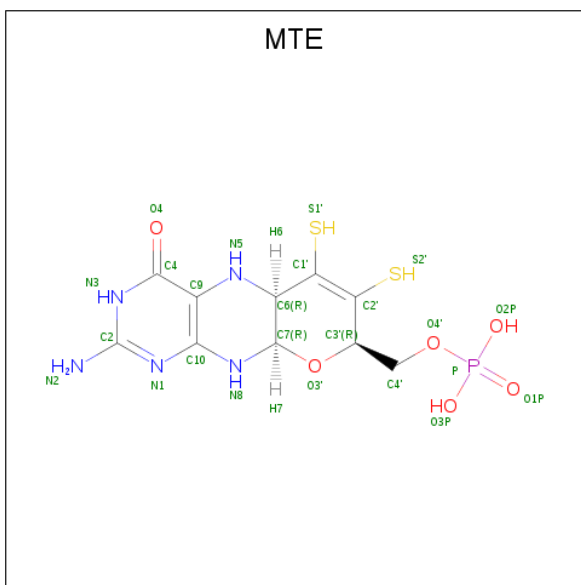
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

- Molecule 3 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe₂S₂).



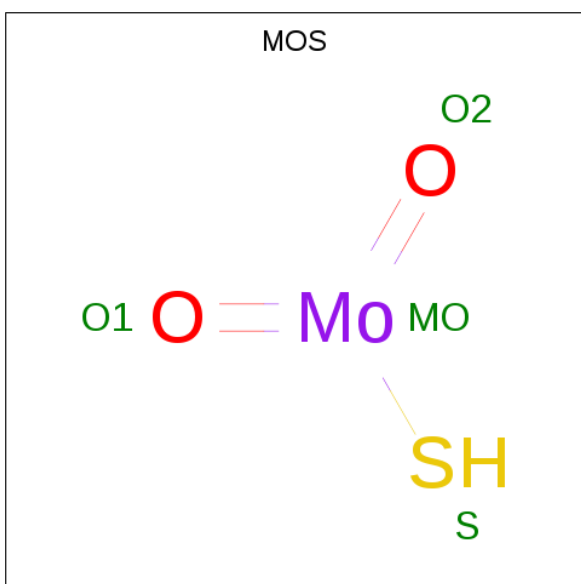
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	A	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	B	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	C	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		
3	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 4 is PHOSPHONIC ACIDMONO-(2-AMINO-5,6-DIMERCAPTO-4-OXO-3,7,8A, 9,10,10A-HEXAHYDRO-4H-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-7-YLMETHYL) ESTER (three-letter code: MTE) (formula: C₁₀H₁₄N₅O₆P₂S₂).



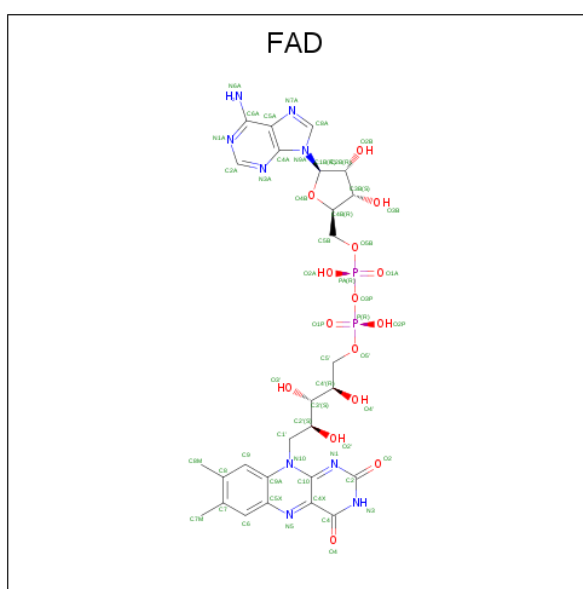
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	B	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	C	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0
4	D	1	Total 24	C 10	N 5	O 6	P 1	S 2	0	0

- Molecule 5 is DIOXOTHIOMOLYBDENUM(VI) ION (three-letter code: MOS) (formula: HMoO_2S).



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

- Molecule 6 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



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

- Molecule 7 is water.

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

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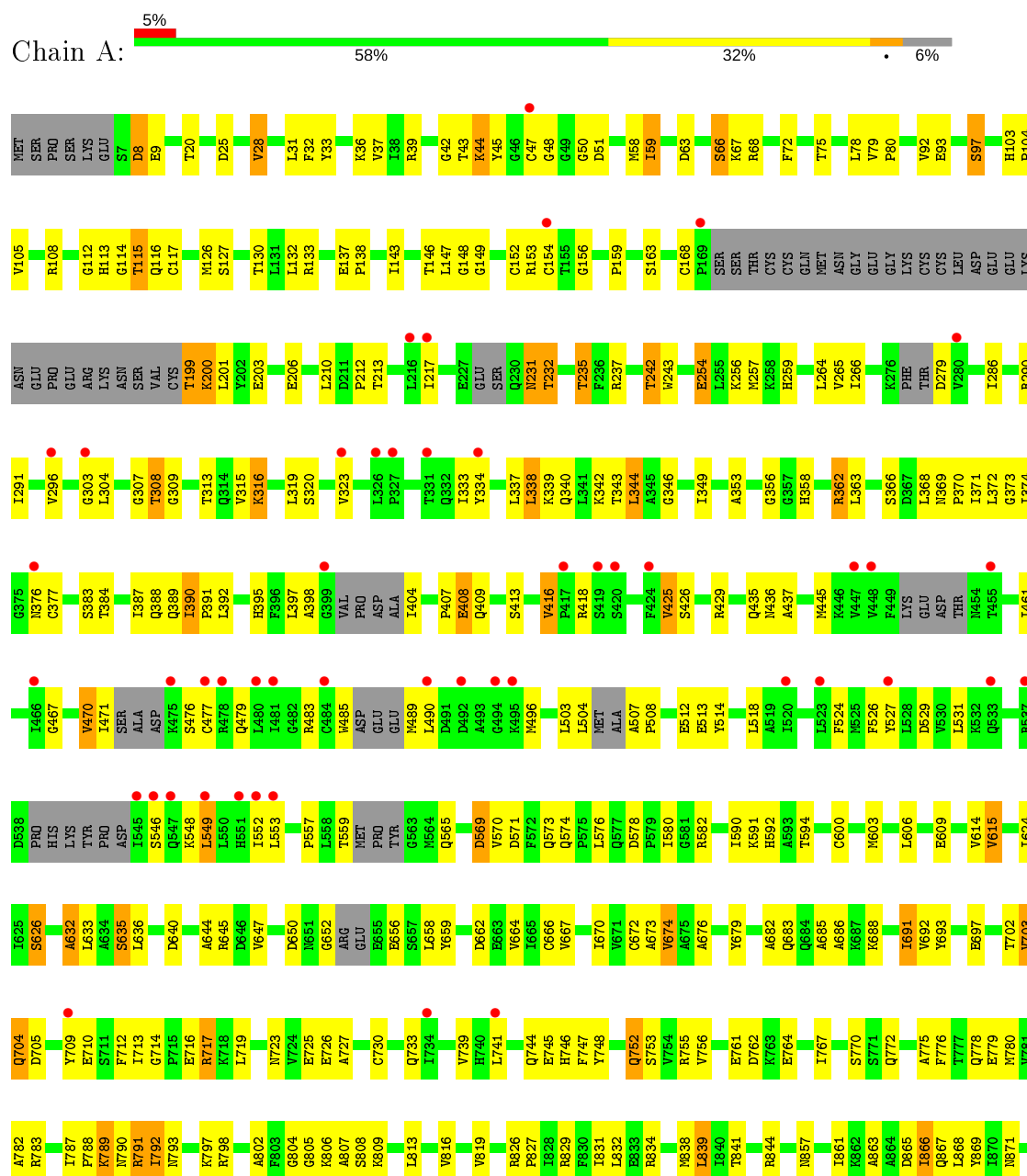
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	166	Total 166	O 166	0	0
7	C	147	Total 147	O 147	0	0
7	D	155	Total 155	O 155	0	0

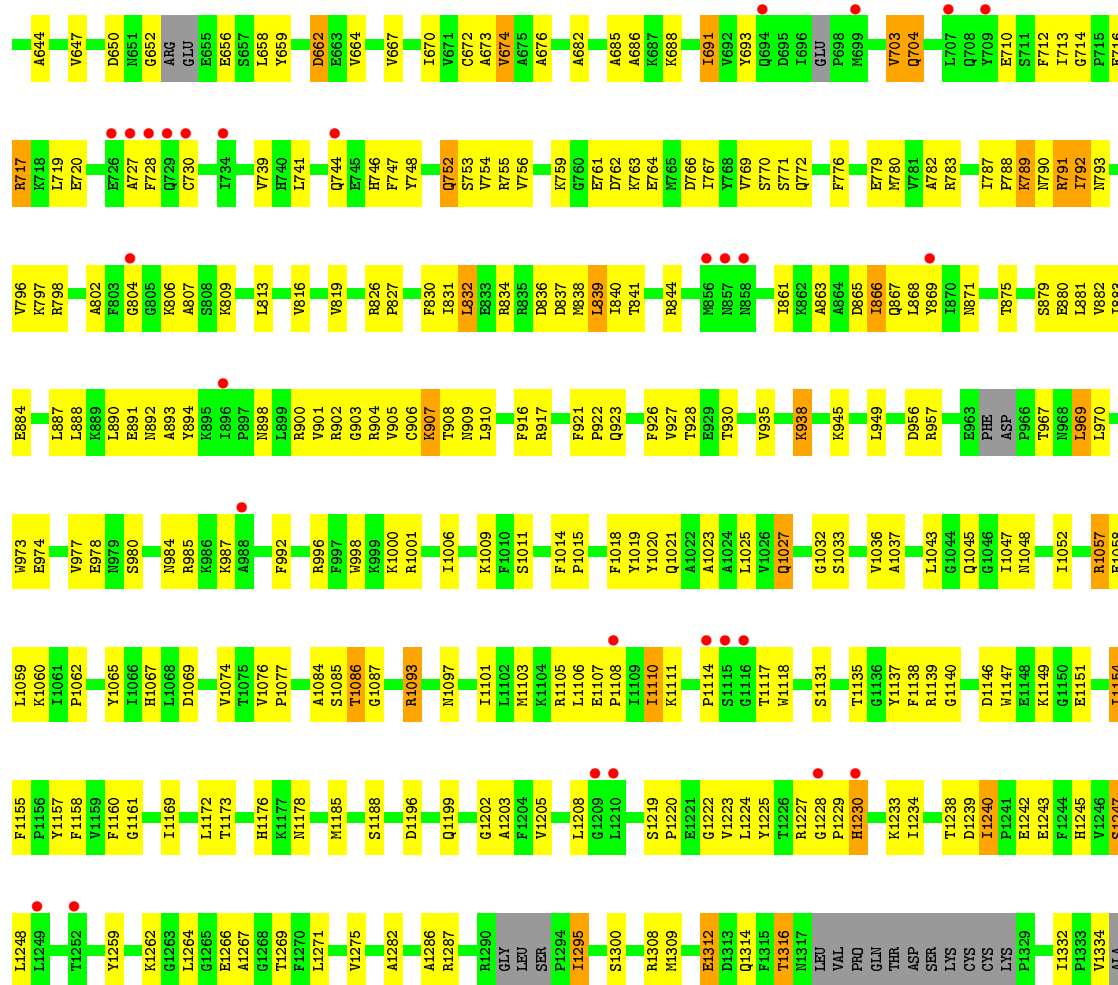
3 Residue-property plots

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

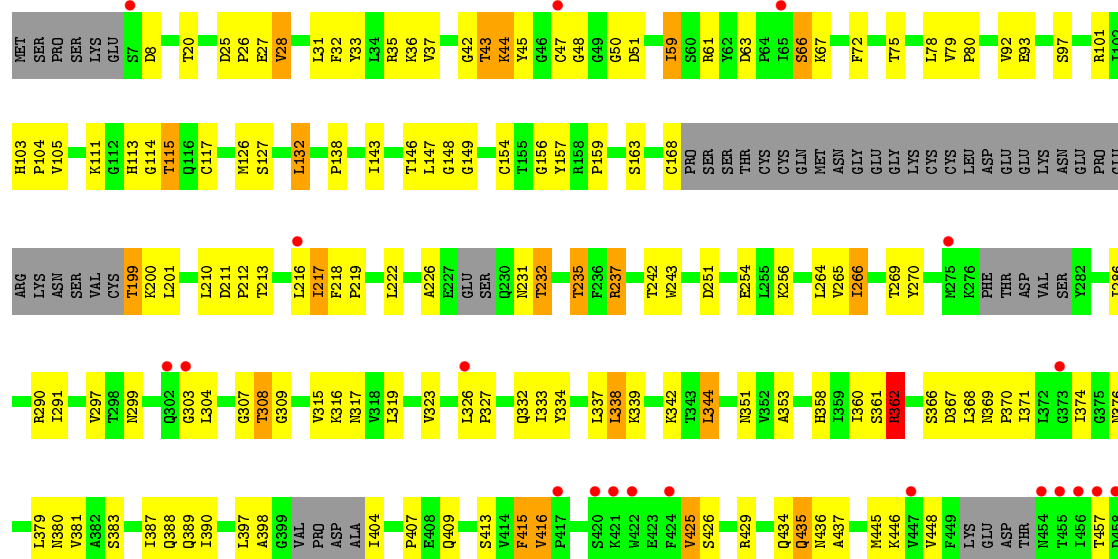
• Molecule 1: AOX3

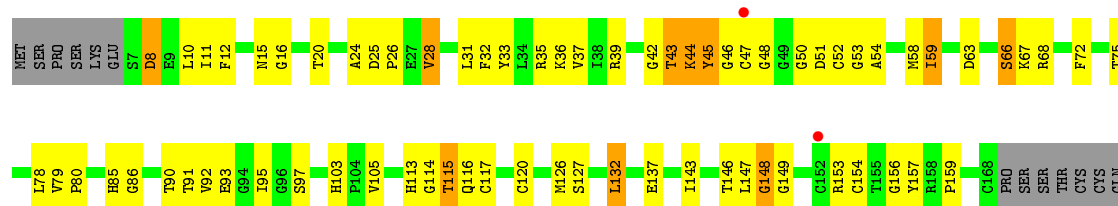






• Molecule 1: AOX3





L1271	F193	N1097	R1001	K907	L913	G737	V667	P579	P508	R433	V352	L264	MET
V1275	D196	T1101	I1006	T908	V619	E738	T670	I580	E512	Q434	A353	L265	ASN
A1282	I1197	L1102	K1009	L910	H740	H740	V671	R582	E513	Q435	S354	I266	GLY
A1286	G1202	K1104	F1010	A915	P826	G742	V674	H566	L514	A437	G357	T269	LYS
R1287	A1203	L1105	S1011	F916	T631	G743	A675	Q587	L518	M445	H358	Y270	CYS
E1288	L1106	L1107	P1015	R917	L332	Q744	A676	S588	A519	K446	I359	L271	LEU
E1289	E1107	P1108	P1015	G918	L332	Q745	A676	G589	I520	V447	S361	H274	ASP
R1290	V1205	P1108	P1015	F919	R834	H746	D677	I590	L523	V448	R362	K276	GLU
GLY	Q1206	I1109	F1018	G920	R834	F747	A682	K591	L523	F449	R362	K277	GLY
LEU	G1207	I1110	F1018	F921	R835	Y748	A682	H592	M525	F449	S366	K278	LYS
SER	L1208	K1111	Q1021	P922	R836	Q752	A685	T594	F526	D452	S366	T278	ASN
I1295	Y1211	Q1112	A1022	Q923	R837	S753	A686	G595	F527	T453	N369	D279	GLU
S1300	S1219	P1113	A1023	V927	L838	V756	G596	E596	L528	T454	P370	V280	PRO
R1308	G1222	S1115	L1025	T928	R340	G760	K688	V605	D529	T455	I371	S281	GLU
E1312	P1220	G1116	V1026	E929	T941	E761	K688	L606	L531	T457	I374	Y282	ARG
D1313	Q1027	T1117	Q1027	T930	G842	E762	L691	E609	K532	D458	I375	I286	LYS
T1316	I1028	W1118	I1028	R944	G843	E763	Y693	V614	Q533	L459	I376	S287	ASN
R1317	Y1127	V1127	L1035	R940	N857	E764	Y693	V615	T536	G460	I378	R290	SER
R1318	S1131	Y1127	V1036	LEU	N858	E764	Y693	V615	R537	L462	I378	I291	VAL
VAL	G1228	T1227	A1037	P942	I767	I767	I696	I624	D538	Y463	S383	V297	CYS
GLN	P1229	G1228	L1043	R945	A863	S770	P688	I625	PRO	G467	S383	V298	T199
THR	R1231	Y1137	G1044	L949	A864	S771	H599	S626	HIS	G467	G396	T299	K200
ASP	K1233	R1139	Q1045	L949	R866	Q772	T702	L627	LYS	V470	G396	T299	L201
SER	I1234	R1140	I1047	D956	Q677	D773	T703	S630	TRP	I471	I390	L304	Y202
LYS	Y1246	Y1141	N1048	R957	Y869	F776	Q704	E631	ASP	I471	I390	L304	F207
P1329	V1237	Q1142	I1052	E963	N871	E779	D705	A632	I545	K475	H395	Q307	L210
T1238	T1238	W1147	A1055	PHE	S879	E780	Q708	A632	S546	S476	H395	Q308	D211
D1239	D1239	K1149	S1056	ASP	E880	A782	E710	A634	Q547	C477	A398	T308	P212
E1243	E1243	G1150	R1057	PRO	L881	R783	E711	S635	K548	Q479	GLY	G309	T213
F1244	F1244	E1151	E1058	T967	V882	E783	F712	L636	L549	L480	VAL	S311	L216
H1245	H1245	G1152	L1059	N968	R883	E783	F712	L636	L550	I481	PRO	V315	I217
V1246	V1246	D1153	K1060	L969	E884	E787	F715	D640	H551	G482	ASP	N317	F218
S1247	S1247	I1154	L970	L970	E884	E787	F715	A644	L553	C484	ALA	I404	L222
T1250	T1250	F1155	I1066	H973	L487	E789	E716	V647	P557	W485	P407	I319	E227
P1251	P1251	Y1157	H1067	E974	L888	E791	R717	V647	LEU	D486	E408	I319	GLU
P1253	P1253	F1158	L1068	E974	R889	E792	E718	D650	THR	E487	Q409	V622	SER
Y1259	Y1259	V1159	D1069	E978	L290	E793	L719	M651	MET	E488	Q409	V623	GLN
K1262	K1262	G1161	V1074	E981	A693	V796	G723	G652	PRO	M489	S413	P327	N231
L1264	L1264	T1075	V1076	E981	A693	K797	N723	ARG	Y562	D492	F414	P327	T232
E1265	E1265	N1178	P1077	S981	Y694	R798	N724	GLU	Q565	A493	V416	I333	T235
E1266	E1266	N1185	G1083	N984	N898	A802	E725	E655	Q568	G494	V416	G395	F236
A1267	A1267	S1188	G1084	N984	L899	F803	E726	E656	S657	K495	S419	I334	R237
G1268	G1268	F1189	A1084	N987	R900	G804	A727	S657	D569	M496	S420	Y334	R240
T1269	T1269	N1178	S1085	N987	V901	G805	F728	L658	V570	I497	K421	K339	T241
F1270	F1270	N1185	T1086	N987	R902	K306	Q729	Y659	D571	C498	E423	P423	T242
			G1087	N987	G903	A807	C730	D662	F572	L503	F424	K342	T243
			R1093	N987	G905	A807	C730	E663	P575	LEU	V425	T343	T243
				N987	V905	A807	C730	V664	L576	MET	S426	L344	F256
				N987	C906	R809	E736	C666	Q577	ALA	R429	N351	H259

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 135.27Å 147.37Å 78.16° 77.72° 89.90°	Depositor
Resolution (Å)	49.91 – 2.54 49.91 – 2.55	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
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.256 , 0.285 0.250 , 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	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	38315	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MOS, NA, FES, FAD, MTE

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(°)	Ideal(°)
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

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:H9	6:C:3005:FAD:H2'	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:HD12	1:B:216:LEU:H	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:C9	6:C:3005:FAD:H2'	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:723:ASN:ND2	7:D:2105:HOH:O	2.06	0.86
1:D:650:ASP:OD2	1:D:783:ARG:NH1	2.07	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:741:LEU:HG	1:B:1300:SER:HB2	1.60	0.84
1:B:650:ASP:OD2	1:B:783:ARG:NH1	2.08	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:1077:PRO:HG3	1:D:1027:GLN:HG3	1.59	0.83
1:C:251:ASP:OD1	7:C:2043:HOH:O	1.96	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:1294:PRO:O	7:D:2153:HOH:O	1.98	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:GLN:NE2	7:D:2082:HOH:O	2.11	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:1094:ALA:HB1	7:C:2119:HOH:O	1.80	0.79
1:C:201:LEU:HD11	1:C:565:GLN:HG3	1.62	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:C9	6:B:3005:FAD:O2'	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:H	1:D:216:LEU:CD1	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:HE21	1:B:704:GLN:H	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:C5B	6:B:3005:FAD:H8A	2.15	0.75
1:D:333:ILE:HG22	1:D:425:VAL:HG11	1.68	0.75
1:A:1097:ASN:HD22	1:A:1137:TYR:H	1.35	0.75
1:A:316:LYS:HG3	7:A:2060:HOH:O	1.86	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:HG3	1:A:1093:ARG:HH11	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:HG3	1:D:1093:ARG:HH11	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:1142:GLN:HG2	7:D:2140:HOH:O	1.88	0.72
1:D:264:LEU:O	6:D:3005:FAD:H2B	1.89	0.72
1:C:1161:GLY:HA3	1:C:1185:MET:HE2	1.71	0.72
1:C:31:LEU:CD2	1:C:45:TYR:HB3	2.19	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:1065:TYR:HB3	7:B:2141:HOH:O	1.90	0.72
1:B:314:GLN:OE1	7:B:2052:HOH:O	2.07	0.72
1:A:1219:SER:OG	1:A:1223:VAL:HG12	1.90	0.71
1:A:130:THR:HG23	7:A:2015:HOH:O	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:340:GLN:HA	7:A:2062:HOH:O	1.90	0.71
1:A:8:ASP:OD1	7:A:2002:HOH:O	2.07	0.71
1:B:1161:GLY:HA3	1:B:1185:MET:HE2	1.71	0.71
1:B:337:LEU:HD23	1:B:371:ILE:HD11	1.72	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:1087:GLY:N	4:B:3003:MTE:O1P	2.24	0.70
1:B:458:ASP:OD1	1:B:459:LEU:N	2.24	0.70
1:B:41:THR:OG1	7:B:2015:HOH:O	2.08	0.70
1:B:31:LEU:CD2	1:B:45:TYR:HB3	2.22	0.70
1:D:630:SER:N	7:D:2090:HOH:O	2.25	0.70
1:C:1015:PRO:HA	1:C:1154:ILE:HG22	1.73	0.69
1:C:337:LEU:HD23	1:C:371:ILE:HD11	1.74	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:1093:ARG:HG3	1:C:1093:ARG:HH11	1.56	0.69
1:C:683:GLN:OE1	7:C:2089:HOH:O	2.09	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: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:B:293:GLU:OE1	7:B:2050:HOH:O	2.11	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:HG2	1:A:1093:ARG:HH11	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:1287:ARG:NH2	7:B:2162:HOH:O	2.27	0.66
1:B:875:THR:O	7:B:2124:HOH:O	2.13	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:1178:ASN:ND2	1:D:1239:ASP:O	2.24	0.66
1:D:15:ASN:ND2	7:D:2004:HOH:O	2.27	0.66
1:B:547:GLN:N	1:B:547:GLN:OE1	2.28	0.66
1:A:108:ARG:O	7:A:2025:HOH:O	2.12	0.66
1:A:1178:ASN:ND2	1:A:1239:ASP:O	2.28	0.66
1:A:809:LYS:HE3	1:A:841:THR:O	1.96	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:892:ASN:O	1:D:1009:LYS:HE3	1.97	0.64
1:D:8:ASP:O	7:D:2001:HOH:O	2.14	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:H	1:B:387:ILE:HD12	1.62	0.64
1:D:58:MET:HB3	7:D:2012:HOH:O	1.98	0.64
1:A:387:ILE:H	1:A:387:ILE:HD12	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:HD1	1:B:415:PHE:C	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: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:A:761:GLU:HG3	1:B:591:LYS:CD	2.30	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:NE2	1:B:704:GLN:H	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:C	1:C:490:LEU:HD23	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:357:GLY:HA3	6:B:3005:FAD:O1P	2.01	0.61
1:B:47:CYS:SG	1:B:48:GLY:N	2.73	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:HD23	1:B:490:LEU:C	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:645:ARG:NH2	7:A:2110:HOH:O	2.33	0.60
1:A:59:ILE:HD11	1:A:72:PHE:CE2	2.36	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:CD1	1:B:415:PHE:C	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:741:LEU:HA	1:B:1300:SER:HB3	1.83	0.60
1:B:590:ILE:O	1:B:594:THR:HG23	2.01	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:367:ASP:HB2	6:C:3005:FAD:O2	2.02	0.60
1:C:59:ILE:HD11	1:C:72:PHE:CE2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ILE:HG13	1:C:72:PHE:CZ	2.37	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:CD1	1:D:415:PHE:C	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: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:591:LYS:CD	1:B:761:GLU:HG3	2.32	0.59
1:A:257:MET:HG2	1:A:384:THR:HG21	1.84	0.59
1:A:59:ILE:HG13	1:A:72:PHE:CZ	2.37	0.59
1:C:381:VAL:N	7:C:2060:HOH:O	2.32	0.59
1:C:50:GLY:HA2	3:C:3002:FES:S2	2.43	0.59
1:A:1103:MET:HA	1:A:1103:MET:HE2	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:1206:GLN:HG3	7:A:2033:HOH:O	2.03	0.58
1:A:741:LEU:HD11	1:A:926:PHE:CD2	2.38	0.58
1:B:1045:GLN:N	1:B:1045:GLN:OE1	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:703:VAL:HG12	1:C:1334:VAL:O	2.03	0.58
1:C:358:HIS:NE2	1:C:366:SER:OG	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:667:VAL:HG22	1:D:667:VAL:O	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:1157:TYR:CE1	1:B:1262:LYS:HG3	2.39	0.58
1:B:727:ALA:HB2	1:B:898:ASN:ND2	2.18	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:667:VAL:HG11	1:A:1222:GLY:O	2.03	0.57
1:A:356:GLY:N	7:A:2058:HOH:O	2.36	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:C8A	6:B:3005:FAD:H52A	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:N	1:C:1045:GLN:OE1	2.33	0.57
1:A:1154:ILE:HD12	1:A:1155:PHE:CZ	2.39	0.57
1:A:719:LEU:HD11	1:A:888:LEU:HD23	1.86	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:1154:ILE:HD12	1:C:1155:PHE:CZ	2.39	0.57
1:C:387:ILE:HD12	1:C:387:ILE:N	2.20	0.57
1:C:507:ALA:HB1	1:C:508:PRO:HD2	1.86	0.57
1: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:1093:ARG:CG	1:A:1093:ARG:NH1	2.57	0.57
1:A:338:LEU:HD21	7:A:2060:HOH:O	2.04	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:1157:TYR:CE1	1:D:1262:LYS:HG3	2.39	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:A:591:LYS:HD3	1:B:761:GLU:HG3	1.87	0.56
1:B:580:ILE:CG1	1:B:1057:ARG:HG3	2.35	0.56
1:D:753:SER:HB3	1:D:831:ILE:HD13	1.87	0.56
1:D:90:THR:HB	7:D:2012:HOH:O	2.04	0.56
1:A:50:GLY:HA2	3:A:3002:FES:S2	2.45	0.56
1:A:782:ALA:HB1	1:A:787:ILE:O	2.05	0.56
1:C:667:VAL:HG11	1:C:1222:GLY:O	2.05	0.56
1:D:580:ILE:CG1	1:D:1057:ARG:HG3	2.36	0.56
1:D:344:LEU:C	1:D:344:LEU:HD12	2.26	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:256:LYS:HE3	1:D:407:PRO:O	2.05	0.56
1:D:50:GLY:HA2	3:D:3002:FES:S2	2.45	0.56
1:A:968:ASN:N	7:A:2148:HOH:O	2.29	0.56
1:C:344:LEU:HD12	1:C:344:LEU:C	2.27	0.56
1:C:415:PHE:HD1	1:C:415:PHE:C	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:N	1:A:387:ILE:HD12	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:1084:ALA:O	1:D:1086:THR:HG22	2.06	0.55
1:D:667:VAL:HG11	1:D:1222:GLY:O	2.07	0.55
1:D:614:VAL:HG12	1:D:673:ALA:HB2	1.89	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:1047:ILE:HG23	7:C:2130:HOH:O	2.07	0.55
1:C:27:GLU:HG3	7:C:2004: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:1093:ARG:NH1	1:B:1093:ARG:CG	2.55	0.55
1:B:154:CYS:O	1:B:1202:GLY:HA3	2.07	0.55
1:C:1103:MET:HE1	1:C:1118:TRP:HZ3	1.71	0.55
1:C:358:HIS:HA	6:C:3005:FAD:O4'	2.07	0.55
1:A:344:LEU:HD12	1:A:344:LEU:C	2.28	0.54
1:C:969:LEU:HB2	1:C:1160:PHE:CD1	2.41	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:D:788:PRO:HG2	1:D:791:ARG:NH1	2.22	0.54
1:A:1023:ALA:HB3	1:A:1076:VAL:HG13	1.89	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:C:1103:MET:HA	1:C:1103:MET:HE2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1137:TYR:CD1	1:D:1131:SER:HB2	2.42	0.54
1:C:713:ILE:HG13	1:C:907:LYS:CB	2.38	0.54
1:C:770:SER:O	1:C:806:LYS:HD3	2.07	0.54
1:C:868:LEU:HD12	1:C:887:LEU:HD23	1.90	0.54
1: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:OD1	1:C:578:ASP:C	2.45	0.54
1:D:756:VAL:O	1:D:827:PRO:HA	2.07	0.54
1:A:1220:PRO:HA	1:A:1332:ILE:HD13	1.90	0.54
1:A:868:LEU:HD12	1:A:887:LEU:HD23	1.90	0.54
1:A:917:ARG:CZ	1:A:1203:ALA:HB2	2.38	0.54
1:C:1311:CYS:HB2	7:C:2136:HOH:O	2.07	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:D:1045:GLN:N	1:D:1045:GLN:OE1	2.33	0.54
1:A:1196:ASP:HB3	1:A:1264:LEU:HD12	1.90	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: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:HG13	1:D:1110:ILE:O	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:1067:HIS:ND1	7:D:2134:HOH:O	2.28	0.53
1:D:383:SER:HB3	1:D:409:GLN:HB3	1.90	0.53
1:D:415:PHE:HD1	1:D:415:PHE:C	2.11	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:1025:LEU:HD13	1:A:1135:THR:HG22	1.91	0.53
1:A:154:CYS:O	1:A:1202:GLY:HA3	2.09	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: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:C:333:ILE:HD11	1:C:416:VAL:HG23	1.90	0.53
1:D:884:GLU:OE1	1:D:1147:TRP:NE1	2.41	0.53
1:D:868:LEU:HD12	1:D:887:LEU:HD23	1.90	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:1018:PHE:O	1:A:1021:GLN:HG2	2.09	0.53
1:A:580:ILE:CG1	1:A:1057:ARG:HG3	2.39	0.53
1:B:969:LEU:HB2	1:B:1160:PHE:CD1	2.43	0.53
1:B:201:LEU:CD1	1:B:565:GLN:HG3	2.35	0.53
1:C:1009:LYS:HD3	1:C:1158:PHE:CD2	2.44	0.53
1:C:303:GLY:HA3	1:C:415:PHE:CE1	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:1111:LYS:O	1:B:1114:PRO:HD3	2.09	0.53
1:B:900:ARG:HH11	1:B:902:ARG:NH2	2.07	0.53
1:C:1084:ALA:O	1:C:1086:THR:HG22	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: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:C	1:D:578:ASP:OD1	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:685:ALA:HA	1:C:688:LYS:HD2	1.91	0.52
1:C:92:VAL:HA	1:C:126:MET:CE	2.39	0.52
1:D:1196:ASP:HB3	1:D:1264:LEU:HD12	1.91	0.52
1:D:32:PHE:CE1	1:D:36:LYS:HG3	2.45	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: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:A:606:LEU:HD23	1:B:606:LEU:HD23	1.91	0.52
1:D:741:LEU:HA	1:D:1300:SER:CB	2.40	0.52
1:D:264:LEU:HD13	1:D:286:ILE:HB	1.92	0.52
1:A:333:ILE:HD11	1:A:416:VAL:HG23	1.90	0.52
1:B:1023:ALA:HB3	1:B:1076:VAL:HG13	1.91	0.52
1:B:33:TYR:HA	1:B:37:VAL:HG12	1.91	0.52
1:C:1103:MET:HA	1:C:1103:MET:CE	2.40	0.52
1:C:483:ARG:NH2	1:C:489:MET:HA	2.25	0.52
1:D:270:TYR:HB3	6:D:3005:FAD:O1A	2.09	0.52
1:A:808:SER:HB3	7:A:2136:HOH:O	2.08	0.52
1:B:1154:ILE:O	7:B:2154:HOH:O	2.18	0.52
1:A:761:GLU:HG3	1:B:591:LYS:HD3	1.92	0.52
1:B:644:ALA:HB2	7:B:2097:HOH:O	2.08	0.52
1:B:75:THR:OG1	7:B:2020:HOH:O	2.03	0.52
1:A:1084:ALA:O	1:A:1086:THR:HG22	2.09	0.52
1:A:371:ILE:HA	1:A:374:ILE:HG22	1.92	0.52
1:A:66:SER:O	1:A:67:LYS:HB2	2.10	0.52
1:A:761:GLU:HG3	1:B:591:LYS:HD2	1.91	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:467:GLY:HA3	1:C:471:ILE:CG2	2.40	0.52
1:C:63:ASP:O	1:C:67:LYS:N	2.40	0.52
1:D:297:VAL:O	1:D:297:VAL:HG13	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:1043:LEU:HG	1:C:1045:GLN:HE22	1.75	0.52
1:C:1000:LYS:HE2	1:C:1286:ALA:HA	1.92	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:D:1101:ILE:O	1:D:1105:ARG:HG3	2.09	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: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:O	1:C:647:VAL:HG23	2.10	0.52
1:D:291:ILE:HD12	1:D:291:ILE:N	2.24	0.52
1:A:1110:ILE:O	1:A:1110:ILE:HG13	2.09	0.52
1:A:308:THR:HG22	1:A:309:GLY:N	2.24	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:1131:SER:HB2	1:D:1137:TYR:CD1	2.44	0.51
1:C:216:LEU:N	1:C:216:LEU:HD12	2.26	0.51
1:C:33:TYR:CD1	1:C:37:VAL:HG11	2.44	0.51
1:D:1009:LYS:HD3	1:D:1158:PHE:CD2	2.45	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: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:1009:LYS:HD3	1:B:1158:PHE:CD2	2.45	0.51
1:B:578:ASP:OD1	1:B:578:ASP:C	2.46	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:1009:LYS:HD3	1:A:1158:PHE:CD2	2.45	0.51
1:A:147:LEU:O	1:A:149:GLY:N	2.42	0.51
1:A:33:TYR:CD1	1:A:37:VAL:HG11	2.44	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:1000:LYS:HE2	1:A:1286:ALA:HA	1.92	0.51
1:A:467:GLY:HA3	1:A:471:ILE:CG2	2.40	0.51
1:A:945:LYS:O	1:A:949:LEU:HG	2.10	0.51
1: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:B:483:ARG:NH2	1:B:489:MET:HA	2.26	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:1067:HIS:HE1	1:D:764:GLU:OE2	1.92	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:61:ARG:NH1	7:C:2010:HOH:O	2.40	0.51
1:D:1069:ASP:N	7:D:2134:HOH:O	2.44	0.51
1:A:1045:GLN:OE1	1:A:1045:GLN:N	2.33	0.51
1:A:291:ILE:N	1:A:291:ILE:HD12	2.26	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:HH11	1:A:798:ARG:HG2	1.76	0.51
1:B:1000:LYS:HE2	1:B:1286:ALA:HA	1.93	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:D:1025:LEU:HD13	1:D:1135:THR:HG22	1.93	0.51
1:D:1093:ARG:HG3	1:D:1093:ARG:NH1	2.23	0.51
1:D:66:SER:O	1:D:67:LYS:HB2	2.11	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:OD1	1:A:578:ASP:C	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:1296:TRP:N	7:A:2176:HOH:O	2.44	0.50
1:A:987:LYS:HD2	7:A:2150:HOH:O	2.12	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:1103:MET:HA	1:A:1103:MET:CE	2.40	0.50
1:A:659:TYR:HE2	1:A:819:VAL:HG21	1.75	0.50
1:C:1093:ARG:CG	1:C:1093:ARG:NH1	2.56	0.50
1:D:1000:LYS:HE2	1:D:1286:ALA:HA	1.92	0.50
1:A:507:ALA:HB1	1:A:508:PRO:HD2	1.93	0.50
1:A:632:ALA:O	1:A:635:SER:N	2.42	0.50
1:A:633:LEU:H	1:A:633:LEU:HD12	1.76	0.50
1:A:793:ASN:HB3	1:A:1074:VAL:CG2	2.42	0.50
1:A:92:VAL:HA	1:A:126:MET:CE	2.38	0.50
1:B:1058:GLU:OE1	1:B:1259:TYR:OH	2.29	0.50
1:B:790:ASN:OD1	1:B:791:ARG:HD3	2.11	0.50
1:B:770:SER:C	7:B:2115:HOH:O	2.39	0.50
1:B:798:ARG:HG2	1:B:798:ARG:HH11	1.76	0.50
1:C:1137:TYR:CG	1:D:1131:SER:HB2	2.47	0.50
1:D:1058:GLU:OE1	1:D:1259:TYR:OH	2.28	0.50
1:D:154:CYS:O	1:D:1202:GLY:HA3	2.11	0.50
1:A:987:LYS:NZ	7:A:2149:HOH:O	2.26	0.50
1:B:793:ASN:HB3	1:B:1074:VAL:CG2	2.41	0.50
1:B:770:SER:N	7:B:2115:HOH:O	2.41	0.50
1:C:614:VAL:HG12	1:C:673:ALA:CB	2.42	0.50
1:C:790:ASN:OD1	1:C:791:ARG:HD3	2.11	0.50
1:C:772:GLN:HE22	1:C:804:GLY:HA2	1.77	0.50
1:D:1103:MET:CE	1:D:1103:MET:HA	2.42	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:B:1025:LEU:HD13	1:B:1135:THR:HG22	1.94	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: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:1103:MET:CE	1:B:1103:MET:HA	2.42	0.50
1:B:307:GLY:HA2	1:B:413:SER:HB3	1.93	0.50
1:C:1023:ALA:HB3	1:C:1076:VAL:HG13	1.93	0.50
1:C:704:GLN:N	1:C:704:GLN:HE21	2.05	0.50
1:C:863:ALA:HA	1:C:898:ASN:O	2.12	0.50
1:D:797:LYS:HG3	1:D:1069:ASP:O	2.12	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:A:1106:LEU:O	1:A:1110:ILE:HG23	2.11	0.49
1:A:308:THR:HG21	6:A:3005:FAD:H62A	1.68	0.49
1:A:33:TYR:HA	1:A:37:VAL:HG12	1.93	0.49
1:A:756:VAL:O	1:A:827:PRO:HA	2.12	0.49
1:B:1097:ASN:ND2	1:B:1137:TYR:H	2.07	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:C:1077:PRO:HD3	1:D:1027:GLN:OE1	2.12	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:D:839:LEU:HG	1:D:1227:ARG:HD3	1.94	0.49
1:D:47:CYS:SG	1:D:48:GLY:N	2.82	0.49
1:A:1058:GLU:OE1	1:A:1259:TYR:OH	2.30	0.49
1:A:955:ILE:HA	7:A:2144:HOH:O	2.12	0.49
1:C:1018:PHE:O	1:C:1021:GLN:HG2	2.12	0.49
1:C:291:ILE:HD12	1:C:291:ILE:N	2.27	0.49
1:C:66:SER:O	1:C:67:LYS:HB2	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:1208:LEU:HD12	1:B:1275:VAL:HG21	1.94	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: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:1018:PHE:O	1:D:1021:GLN:HG2	2.13	0.49
1:D:1048:ASN:O	1:D:1052:ILE:HG12	2.12	0.49
1:D:1023:ALA:HB3	1:D:1076:VAL:HG13	1.93	0.49
1:D:33:TYR:CD1	1:D:37:VAL:HG11	2.47	0.49
1:A:1101:ILE:O	1:A:1105:ARG:HG3	2.12	0.49
1:A:307:GLY:HA2	1:A:413:SER:HB3	1.93	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:1314:GLN:CD	1:A:1314:GLN:H	2.15	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: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:1143:ALA:HB2	7:C:2132:HOH:O	2.11	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:42:GLY:O	1:C:44:LYS:HE3	2.12	0.49
1:C:580:ILE:HG13	1:C:1057:ARG:HG3	1.95	0.49
1:D:1208:LEU:HD12	1:D:1275:VAL:HG21	1.93	0.49
1:D:580:ILE:HG13	1:D:1057:ARG:HG3	1.94	0.49
1:A:1219:SER:OG	1:A:1223:VAL:CG1	2.59	0.49
1:B:1101:ILE:O	1:B:1105:ARG:HG3	2.13	0.49
1:B:667:VAL:HB	7:B:2103:HOH:O	2.11	0.49
1:B:153:ARG:HH22	1:B:744:GLN:HE21	1.60	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: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:C:804:GLY:HA2	5:C:3004:MOS:O1	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: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:1111:LYS:HD3	1:A:1111:LYS:HA	1.67	0.49
1:A:1227:ARG:NH2	7:A:2173:HOH:O	2.45	0.49
1:A:32:PHE:CE1	1:A:36:LYS:HG3	2.48	0.49
1:A:770:SER:O	1:A:806:LYS:HD3	2.13	0.49
1:A:753:SER:HB3	1:A:831:ILE:CD1	2.43	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:B:47:CYS:SG	1:B:1229:PRO:HG2	2.52	0.49
1:B:265:VAL:O	1:B:265:VAL:HG13	2.13	0.49
1:B:559:THR:CB	1:B:1242:GLU:HB3	2.43	0.49
1:B:676:ALA:HB3	1:B:682:ALA:HB2	1.94	0.49
1:B:609:GLU:HA	1:B:827:PRO:HG2	1.95	0.49
1:B:712:PHE:CG	1:B:904:ARG:HD3	2.47	0.49
1:C:772:GLN:HE21	1:C:807:ALA:HB2	1.78	0.49
1:D:1152:GLY:HA2	7:D:2142:HOH:O	2.13	0.49
1:D:486:ASP:N	1:D:486:ASP:OD1	2.46	0.49
1:C:761:GLU:HG3	1:D:591:LYS:HD2	1.95	0.49
1:A:137:GLU:OE1	1:D:68:ARG:NH2	2.46	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:1106:LEU:O	1:C:1110:ILE:HG23	2.13	0.48
1:C:78:LEU:O	1:C:80:PRO:HD3	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:772:GLN:NE2	1:B:807:ALA:HB2	2.29	0.48
1:B:770:SER:O	1:B:806:LYS:HD3	2.13	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:1103:MET:HA	1:D:1103:MET:HE2	1.96	0.48
1:D:33:TYR:HA	1:D:37:VAL:HG12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:LYS:HE2	1:D:44:LYS:HB3	1.74	0.48
1:B:33:TYR:O	1:B:37:VAL:HG12	2.13	0.48
1:B:772:GLN:HE22	1:B:804:GLY:HA2	1.77	0.48
1:B:772:GLN:HE21	1:B:807:ALA:HB2	1.78	0.48
1:B:839:LEU:HG	1:B:1227:ARG:HD3	1.94	0.48
1:C:1208:LEU:HD12	1:C:1275:VAL:HG21	1.94	0.48
1:C:888:LEU:HD13	1:C:1154:ILE:CD1	2.43	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:839:LEU:HG	1:A:1227:ARG:HD3	1.95	0.48
1:A:772:GLN:NE2	1:A:807:ALA:HB2	2.28	0.48
1:B:1043:LEU:HG	1:B:1045:GLN:HE22	1.78	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:D:16:GLY:N	7:D:2003:HOH:O	2.12	0.48
1:A:353:ALA:HB1	6:A:3005:FAD:H4'	1.95	0.48
1:A:33:TYR:O	1:A:37:VAL:HG12	2.13	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:NH1	1:B:1093:ARG:HG3	2.23	0.48
1:C:1219:SER:OG	1:C:1223:VAL:CG1	2.62	0.48
1:C:741:LEU:HA	1:C:1300:SER:CB	2.44	0.48
1:C:344:LEU:HD13	6:C:3005:FAD:C10	2.43	0.48
1:C:767:ILE:HD12	1:C:792:ILE:HD12	1.96	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:1196:ASP:HB3	1:C:1264:LEU:HD12	1.96	0.48
1:C:636:LEU:N	7:C:2082:HOH:O	2.47	0.48
1:D:51:ASP:HB3	1:D:1229:PRO:HB2	1.96	0.48
1:A:741:LEU:HA	1:A:1300:SER:CB	2.42	0.48
1:A:78:LEU:O	1:A:80:PRO:HD3	2.14	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:1238:THR:OG1	7:D:2072:HOH:O	2.02	0.48
1:D:58:MET:CG	7:D:2013:HOH:O	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:798:ARG:NH1	1:D:798:ARG:HG2	2.28	0.48
1:A:265:VAL:HG13	1:A:265:VAL:O	2.13	0.48
1:C:659:TYR:HE2	1:C:819:VAL:HG21	1.77	0.48
1:D:1106:LEU:O	1:D:1110:ILE:HG23	2.14	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: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: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:B:36:LYS:HE3	7:B:2010:HOH:O	2.13	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:772:GLN:NE2	1:D:807:ALA:HB2	2.29	0.47
1:D:753:SER:HB3	1:D:831:ILE:CD1	2.43	0.47
1:A:1023:ALA:HB3	1:A:1076:VAL:CG1	2.45	0.47
1:A:390:ILE:HB	7:A:2069:HOH:O	2.14	0.47
1:A:63:ASP:O	1:A:67:LYS:N	2.37	0.47
1:B:78:LEU:O	1:B:80:PRO:HD3	2.14	0.47
1:C:1138:PHE:CE2	1:C:1140:GLY:HA2	2.49	0.47
1:C:839:LEU:HG	1:C:1227:ARG:HD3	1.96	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: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:1018:PHE:O	1:B:1021:GLN:HG2	2.14	0.47
1:B:779:GLU:HB3	1:B:789:LYS:HE3	1.96	0.47
1:B:746:HIS:HA	1:B:916:PHE:CE2	2.50	0.47
1:C:727:ALA:HA	1:C:730:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:719:LEU:CD1	1:C:888:LEU:HD23	2.44	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:549:LEU:HD23	7:A:2086:HOH:O	2.13	0.47
1:A:153:ARG:HH22	1:A:744:GLN:HE21	1.62	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:103:HIS:CE1	1:A:105:VAL:HG23	2.49	0.47
1:A:319:LEU:HB3	1:A:338:LEU:CD2	2.43	0.47
1:A:746:HIS:HA	1:A:916:PHE:CZ	2.50	0.47
1:B:1219:SER:OG	1:B:1223:VAL:CG1	2.61	0.47
1:B:47:CYS:CB	1:B:1229:PRO:HG2	2.43	0.47
1:B:712:PHE:HB3	1:B:904:ARG:HH11	1.80	0.47
1:A:68:ARG:NH2	1:D:137:GLU:OE1	2.47	0.47
1:A:199:THR:OG1	1:A:200:LYS:N	2.47	0.47
1:A:319:LEU:O	1:A:323:VAL:HG22	2.15	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:1314:GLN:H	1:B:1314:GLN:CD	2.18	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:552:ILE:HG22	1:B:998:TRP:CB	2.45	0.47
1:C:374:ILE:HG13	1:C:446:LYS:HB3	1.96	0.47
1:C:633:LEU:H	1:C:633:LEU:HD12	1.78	0.47
1:C:779:GLU:HB3	1:C:789:LYS:HE3	1.96	0.47
1:A:242:THR:HG22	1:A:242:THR:O	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: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:D:713:ILE:CG1	1:D:907:LYS:HB3	2.30	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:888:LEU:HD13	1:B:1154:ILE:CD1	2.44	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:D:1239:ASP:OD1	7:D:2072:HOH:O	2.20	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:33:TYR:O	1:D:37:VAL:CG1	2.63	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:1172:LEU:O	1:C:1308:ARG:NE	2.48	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:D:408:GLU:HG3	1:D:408:GLU:H	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:741:LEU:HA	1:B:1300:SER:CB	2.43	0.46
1:B:143:ILE:O	1:B:146:THR:HG22	2.15	0.46
1:B:387:ILE:CD1	1:B:387:ILE:H	2.28	0.46
1:B:370:PRO:HG3	1:B:470:VAL:HG11	1.98	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:793:ASN:HB3	1:D:1074:VAL:CG2	2.45	0.46
1:D:39:ARG:HB3	7:D:2009:HOH:O	2.14	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:1219:SER:HB3	1:D:1225:TYR:CZ	2.50	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:A:1025:LEU:HD13	1:A:1135:THR:CG2	2.45	0.46
1:A:591:LYS:HD2	1:B:761:GLU:HG3	1.97	0.46
1:B:1146:ASP:OD2	1:B:1149:LYS:HB2	2.16	0.46
1:B:916:PHE:C	5:B:3004:MOS:S	2.94	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

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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:1093:ARG:HD2	7:A:2167:HOH:O	2.16	0.46
1:A:319:LEU:HA	1:A:319:LEU:HD12	1.74	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:1023:ALA:HB3	1:D:1076:VAL:CG1	2.46	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: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
6:C:3005:FAD:H9	6:C:3005:FAD:O3'	2.15	0.46
1:C:703:VAL:HG13	1:C:704:GLN:HE22	1.80	0.46
1:D:46:GLY:O	1:D:834:ARG:NE	2.38	0.46
1:D:633:LEU:HD12	1:D:633:LEU:H	1.79	0.46
1:D:153:ARG:HH22	1:D:744:GLN:HE21	1.63	0.46
1:A:802:ALA:HB3	1:A:1043:LEU:HD13	1.96	0.46
1:C:1314:GLN:CD	1:C:1314:GLN:H	2.18	0.46
1:C:772:GLN:NE2	1:C:807:ALA:HB2	2.31	0.46
1:C:992:PHE:CZ	1:C:996:ARG:HG3	2.50	0.46
1:C:1027:GLN:OE1	1:D:1077:PRO:HD3	2.14	0.46
1:A:844:ARG:NH1	1:A:916:PHE:HB3	2.31	0.46
1:B:804:GLY:HA2	5:B:3004:MOS:O1	2.16	0.46
1:C:986:LYS:CB	7:C:2114:HOH:O	2.64	0.46
1:D:259:HIS:ND1	7:D:2047:HOH:O	2.20	0.46
1:D:970:LEU:O	1:D:974:GLU:HG2	2.16	0.46
1:A:1131:SER:HB2	1:B:1137:TYR:CD1	2.51	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:B:1014:PHE:O	1:B:1020:TYR:OH	2.26	0.46
1:B:319:LEU:O	1:B:323:VAL:HG22	2.16	0.46
1:B:980:SER:HB2	1:B:985:ARG:HH21	1.81	0.46
1:C:606:LEU:HD23	1:D:606:LEU:HD23	1.97	0.46
1:D:143:ILE:O	1:D:146:THR:HG22	2.16	0.46
1:D:271:LEU:O	1:D:275:MET:HB2	2.15	0.46

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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:1021:GLN:HA	1:C:1138:PHE:O	2.15	0.45
1:C:844:ARG:NH2	1:C:916:PHE:CD1	2.83	0.45
1:D:888:LEU:HD13	1:D:1154:ILE:CD1	2.46	0.45
1:D:727:ALA:HA	1:D:730:CYS:SG	2.56	0.45
1:D:75:THR:O	1:D:79:VAL:HG23	2.15	0.45
1:A:659:TYR:CE2	1:A:819:VAL:HG21	2.51	0.45
1:A:66:SER:O	1:A:67:LYS:CB	2.64	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: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: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: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:719:LEU:CD1	1:B:888:LEU:HD23	2.46	0.45
1:B:712:PHE:CB	1:B:904:ARG:NH1	2.80	0.45
1:B:879:SER:HB3	1:B:905:VAL:HG11	1.99	0.45
1:C:1097:ASN:ND2	1:C:1137:TYR:H	2.08	0.45
1:C:667:VAL:HG11	1:C:1223:VAL:HA	1.99	0.45
1:C:792:ILE:HG12	1:C:792:ILE:O	2.17	0.45
1:C:839:LEU:HD23	1:C:839:LEU:HA	1.86	0.45
1:D:1025:LEU:HD13	1:D:1135:THR:CG2	2.46	0.45
1:D:10:LEU:HD22	7:D:2020:HOH:O	2.16	0.45
1:D:1138:PHE:CE2	1:D:1140:GLY:HA2	2.52	0.45
1:D:317:ASN:ND2	7:D:2059:HOH:O	2.48	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:712:PHE:HB3	1:D:904:ARG:HH11	1.81	0.45
1:D:719:LEU:CD1	1:D:888:LEU:HD23	2.47	0.45
1:D:746:HIS:HA	1:D:916:PHE:CZ	2.51	0.45
1:A:113:HIS:C	1:A:115:THR:H	2.20	0.45
1:A:42:GLY:O	1:A:44:LYS:HE3	2.17	0.45
1:A:580:ILE:HG12	1:A:1057:ARG:HG3	1.99	0.45
1:A:719:LEU:CD1	1:A:888:LEU:HD23	2.46	0.45
1:A:1027:GLN:OE1	1:B:1077:PRO:HD3	2.17	0.45
1:B:1169:ILE:HG12	1:B:1282:ALA:HB1	1.98	0.45
1:B:474:ASP:HA	1:B:477:CYS:SG	2.57	0.45
1:B:50:GLY:HA2	3:B:3002:FES:S2	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:C:319:LEU:HB3	1:C:338:LEU:HD23	1.99	0.45
1:C:44:LYS:HB3	1:C:44:LYS:HE2	1.74	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:1097:ASN:ND2	1:A:1137:TYR:H	2.09	0.45
1:A:980:SER:HB2	1:A:985:ARG:HH21	1.81	0.45
1:C:1011:SER:HB3	1:C:1158:PHE:CD2	2.52	0.45
1:C:319:LEU:HD12	1:C:319:LEU:HA	1.76	0.45
1:C:319:LEU:O	1:C:323:VAL:HG13	2.16	0.45
1:D:358:HIS:CB	6:D:3005:FAD:O4'	2.65	0.45
1:D:66:SER:O	1:D:67:LYS:CB	2.65	0.45
1:D:879:SER:HB3	1:D:905:VAL:HG11	1.98	0.45
1:A:804:GLY:HA2	5:A:3004:MOS:O1	2.16	0.45
1:A:798:ARG:NH1	1:A:798:ARG:HG2	2.31	0.45
1:B:1219:SER:HB3	1:B:1225:TYR:CZ	2.52	0.45
1:B:816:VAL:O	1:B:819:VAL:HG22	2.17	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: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:85:HIS:CA	7:D:2002:HOH:O	2.59	0.45
1:D:890:LEU:HD12	1:D:891:GLU:N	2.32	0.45
1:A:1172:LEU:O	1:A:1308:ARG:NE	2.50	0.45
1:A:712:PHE:HB3	1:A:904:ARG:NH1	2.31	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:1006:ILE:HD11	1:D:1271:LEU:HA	1.99	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:58:MET:N	7:D:2012:HOH:O	2.49	0.45
1:D:659:TYR:CE2	1:D:819:VAL:HG21	2.52	0.45
1:A:844:ARG:HG2	1:A:923:GLN:NE2	2.32	0.44
1:B:1021:GLN:HA	1:B:1138:PHE:O	2.18	0.44
1:B:659:TYR:CE2	1:B:819:VAL:HG21	2.51	0.44
1:C:1243:GLU:HG2	1:C:1245:HIS:HE2	1.82	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:NH1	1:C:798:ARG:HG2	2.32	0.44
1:C:879:SER:HB3	1:C:905:VAL:HG11	1.97	0.44
1:D:1172:LEU:O	1:D:1308:ARG:NE	2.50	0.44
1:D:667:VAL:HG11	1:D:1223:VAL:HA	1.99	0.44
1:D:86:GLY:N	7:D:2002:HOH:O	2.45	0.44
1:A:1011:SER:HB3	1:A:1158:PHE:CD2	2.52	0.44
1:A:435:GLN:HG2	1:A:436:ASN:N	2.32	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: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: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: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:1185:MET:SD	1:B:1267:ALA:HB1	2.58	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:C:1219:SER:HB3	1:C:1225:TYR:CZ	2.52	0.44
1:C:1185:MET:SD	1:C:1267:ALA:HB1	2.57	0.44
1:D:232:THR:H	1:D:290:ARG:HH22	1.65	0.44
1:D:916:PHE:C	5:D:3004:MOS:S	2.96	0.44
1:D:723:ASN:HB2	7:D:2105:HOH:O	2.17	0.44
1:A:909:ASN:O	7:A:2117:HOH:O	2.21	0.44
1:A:910:LEU:CD1	1:A:1334:VAL:HG11	2.47	0.44
1:A:950:ASN:N	7:A:2143:HOH:O	2.50	0.44
1:B:1172:LEU:O	1:B:1308:ARG:NE	2.50	0.44
1:B:1006:ILE:HD11	1:B:1271:LEU:HA	1.99	0.44
1:B:712:PHE:HB3	1:B:904:ARG:NH1	2.33	0.44
1:C:1169:ILE:HG12	1:C:1282:ALA:HB1	2.00	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: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:B:319:LEU:O	1:B:323:VAL:HG13	2.17	0.44
1:A:1067:HIS:HE1	1:B:764:GLU:OE2	2.00	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:1023:ALA:HB3	1:C:1076:VAL:CG1	2.48	0.44
1:C:111:LYS:HB3	7:C:2020:HOH:O	2.17	0.44
1:C:485:TRP:O	1:C:485:TRP:CD1	2.71	0.44
1:D:1169:ILE:HG12	1:D:1282:ALA:HB1	2.00	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: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:360:ILE:HG13	6:D:3005:FAD:N3A	2.32	0.44
1:D:362:ARG:HB3	7:D:2064:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:THR:N	7:D:2004:HOH:O	2.31	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:HB3	1:B:44:LYS:HE2	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:1252:THR:HG21	7:D:2125:HOH:O	2.18	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: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: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:C:51:ASP:OD1	1:C:51:ASP:O	2.36	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:767:ILE:CD1	1:C:792:ILE:HD12	2.49	0.43
1:C:746:HIS:HA	1:C:916:PHE:CE2	2.53	0.43
1:D:1021:GLN:HA	1:D:1138:PHE:O	2.18	0.43
1:D:429:ARG:NH2	1:D:437:ALA:O	2.52	0.43
1:B:1138:PHE:CE2	1:B:1140:GLY:HA2	2.53	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:C:1036:VAL:HG12	1:C:1037:ALA:N	2.34	0.43
1:C:969:LEU:HA	1:C:1160:PHE:HB3	2.00	0.43
1:C:1334:VAL:HG12	1:C:1334:VAL:O	2.18	0.43
1:A:1203:ALA:O	1:A:1269:THR:HA	2.19	0.43
1:A:1185:MET:SD	1:A:1267:ALA:HB1	2.58	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:1025:LEU:HD13	1:C:1135:THR:CG2	2.49	0.43
1:C:435:GLN:HG2	1:C:436:ASN:N	2.34	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:D:275:MET:CG	1:D:282:TYR:CE2	3.01	0.43
1:A:1332:ILE:HG13	1:A:1332:ILE:O	2.18	0.43
1:A:44:LYS:HE2	1:A:44:LYS:HB3	1.72	0.43
1:A:51:ASP:O	1:A:51:ASP:OD1	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: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:319:LEU:HB3	1:D:338:LEU:HD23	2.01	0.43
1:D:42:GLY:O	1:D:44:LYS:HE3	2.18	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:1243:GLU:HG2	1:A:1245:HIS:HE2	1.84	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:HG12	1:A:792:ILE:O	2.19	0.43
1:B:938:LYS:NZ	1:B:1295:ILE:HD13	2.31	0.43
1:B:319:LEU:HA	1:B:319:LEU:HD12	1.76	0.43
1:B:562:TYR:C	1:B:562:TYR:CD1	2.92	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: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: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:92:VAL:HG12	1:D:93:GLU:OE1	2.19	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:O	1:B:792:ILE:HG12	2.19	0.43
1:B:984:ASN:ND2	7:B:2135:HOH:O	2.47	0.43
1:C:485:TRP:CE2	7:C:2066:HOH:O	2.69	0.43
1:C:506:ALA:CB	1:C:512:GLU:CG	2.97	0.43
1:C:624:ILE:HD11	1:C:664:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1332:ILE:O	1:D:1332:ILE:HG13	2.19	0.43
1:A:1202:GLY:O	1:A:1205:VAL:N	2.50	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:B:1025:LEU:HD13	1:B:1135:THR:CG2	2.49	0.43
1:B:518:LEU:HD21	1:B:1173:THR:HA	2.00	0.43
1:B:1220:PRO:HA	1:B:1332:ILE:CD1	2.48	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:25:ASP:HB3	1:B:28:VAL:HG12	2.01	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:C:1243:GLU:HG2	1:C:1245:HIS:NE2	2.34	0.43
1:C:33:TYR:CE1	1:C:37:VAL:HG11	2.54	0.43
1:D:333:ILE:HA	1:D:425:VAL:HG21	2.01	0.43
1:A:969:LEU:HA	1:A:1160:PHE:HB3	2.00	0.42
1:A:702:THR:O	1:A:705:ASP:HB2	2.19	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: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:C:893:ALA:HB1	1:C:969:LEU:HD11	1.99	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:D:879:SER:O	1:D:882:VAL:HB	2.19	0.42
1:D:712:PHE:HB3	1:D:904:ARG:NH1	2.34	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: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:72:PHE:HD2	1:C:351:ASN:HB3	1.84	0.42
1:C:387:ILE:H	1:C:387:ILE:CD1	2.30	0.42
1:D:1036:VAL:HG12	1:D:1037:ALA:N	2.32	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:A:992:PHE:CE1	1:A:1001:ARG:HG3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:THR:HG23	1:A:1253:PRO:HD2	2.02	0.42
1:A:356:GLY:CA	7:A:2058:HOH:O	2.67	0.42
1:A:717:ARG:HD3	1:A:884:GLU:HG2	2.01	0.42
1:A:97:SER:HB2	7:A:2022:HOH:O	2.20	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:HA	1:D:222:LEU:HD23	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:1012:VAL:O	1:C:1156:PRO:HD2	2.19	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:D:1219:SER:OG	1:D:1223:VAL:CG1	2.63	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:A:1021:GLN:HA	1:A:1138:PHE:O	2.20	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: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:1006:ILE:HD11	1:C:1271:LEU:HA	2.01	0.42
1:C:25:ASP:HA	1:C:26:PRO:HD3	1.88	0.42
1:D:50:GLY:CA	3:D:3002:FES:S2	3.08	0.42
1:D:35:ARG:HD2	1:D:43:THR:O	2.20	0.42
1:D:880:GLU:O	1:D:884:GLU:HG3	2.20	0.42
1:D:844:ARG:HG2	1:D:923:GLN:NE2	2.34	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: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:C:115:THR:HG23	1:C:592:HIS:ND1	2.35	0.42
1:C:132:LEU:HA	1:C:132:LEU:HD12	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:1220:PRO:HA	1:D:1332:ILE:CD1	2.49	0.42
1:D:299:ASN:CG	1:D:299:ASN:O	2.58	0.42
1:D:269:THR:OG1	6:D:3005:FAD:O2P	2.38	0.42
1:D:72:PHE:HD2	1:D:351:ASN:HB3	1.84	0.42
1:D:836:ASP:O	1:D:840:ILE:HG13	2.19	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:1085:SER:OG	1:A:1266:GLU:HG3	2.19	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:B:1202:GLY:O	1:B:1205:VAL:N	2.52	0.42
1:B:387:ILE:CG2	1:B:388:GLN:N	2.82	0.42
1:B:485:TRP:CD1	1:B:485:TRP:O	2.72	0.42
1:B:883:ILE:HD12	1:B:883:ILE:HA	1.90	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:1043:LEU:HG	1:A:1045:GLN:HE22	1.84	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: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: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:C:1062:PRO:HD2	1:C:1065:TYR:CD1	2.55	0.42
1:C:463:TYR:O	1:C:470:VAL:HG12	2.20	0.42
1:D:868:LEU:HD11	1:D:890:LEU:CD2	2.49	0.42
1:A:1243:GLU:HG2	1:A:1245:HIS:NE2	2.35	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: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:1230:HIS:CD2	1:D:1230:HIS:N	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ALA:CB	1:A:1066:ILE:HD13	2.50	0.41
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: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:O	1:D:374:ILE:HG13	2.20	0.41
1:A:775:ALA:O	1:A:778:GLN:HB3	2.20	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
7:A:2162:HOH:O	1:B:759:LYS:CE	2.63	0.41
1:C:1018:PHE:HB3	1:D:1127:VAL:O	2.19	0.41
1:C:374:ILE:HG13	1:C:374:ILE:O	2.21	0.41
1:D:113:HIS:C	1:D:115:THR:H	2.23	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: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:A:1105:ARG:NH1	1:A:1131:SER:O	2.53	0.41
1:A:709:TYR:O	1:A:710:GLU:C	2.59	0.41
1:B:1243:GLU:HG2	1:B:1245:HIS:NE2	2.35	0.41
1:B:1332:ILE:O	1:B:1332:ILE:HG13	2.20	0.41
1:C:1078:ASN:OD1	1:D:1029:TYR:HA	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: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:1230:HIS:N	1:B:1230:HIS:CD2	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1055:ALA:CB	1:C:1066:ILE:HD13	2.50	0.41
1:C:138:PRO:O	1:C:168:CYS:HB3	2.20	0.41
1:C:426:SER:HB2	1:C:526:PHE:CD1	2.56	0.41
1:C:762:ASP:OD2	1:D:591:LYS:NZ	2.52	0.41
1:C:816:VAL:O	1:C:819:VAL:HG22	2.21	0.41
1: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: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:A:1036:VAL:HG12	1:A:1037:ALA:N	2.34	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: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: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:51:ASP:O	1:B:51:ASP:OD1	2.39	0.41
1:B:992:PHE:CE1	1:B:996:ARG:HG3	2.54	0.41
1:C:1107:GLU:HB3	1:C:1108:PRO:CD	2.51	0.41
1:C:1230:HIS:CD2	1:C:1230:HIS:N	2.89	0.41
1:C:361:SER:O	1:C:362:ARG:C	2.58	0.41
1:D:1035:LEU:CD1	7:D:2134:HOH:O	2.68	0.41
1:D:463:TYR:O	1:D:470:VAL:HG12	2.21	0.41
1:D:52:CYS:O	1:D:54:ALA:N	2.54	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:1107:GLU:N	1:D:1108:PRO:HD2	2.36	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:90:THR:N	7:D:2012:HOH:O	2.46	0.41
1:A:1161:GLY:O	1:A:1162:ALA:HB2	2.21	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:B:1062:PRO:HD2	1:B:1065:TYR:CD1	2.56	0.41
1:B:1161:GLY:HA3	1:B:1185:MET:CE	2.48	0.41
1:B:422:TRP:CG	1:B:451:GLU:HA	2.56	0.41
1:B:448:VAL:O	1:B:457:THR:HB	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:ILE:O	1:C:1005:ILE:HG23	2.21	0.41
1:D:264:LEU:HD22	1:D:264:LEU:N	2.35	0.41
1:D:826:ARG:HB3	1:D:826:ARG:HE	1.64	0.41
1:A:103:HIS:CG	1:A:104:PRO:HD2	2.55	0.41
1:A:834:ARG:O	1:A:838:MET:HG3	2.20	0.41
1:A:880:GLU:N	1:A:880:GLU:CD	2.74	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:33:TYR:CE1	1:B:37:VAL:HG11	2.56	0.41
1:C:353:ALA:HB1	6:C:3005:FAD:H4'	2.02	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:D:291:ILE:N	1:D:291:ILE:CD1	2.84	0.41
1:D:868:LEU:HD12	1:D:887:LEU:CD2	2.50	0.41
1: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: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:HB3	1:A:826:ARG:HE	1.65	0.41
1:B:868:LEU:O	1:B:903:GLY:HA2	2.21	0.41
1:C:1294:PRO:O	1:C:1295:ILE:C	2.59	0.41
1:C:222:LEU:HD23	1:C:222:LEU:HA	1.78	0.41
1:C:297:VAL:O	1:C:297:VAL:HG13	2.21	0.41
1:C:269:THR:OG1	6:C:3005:FAD:O2P	2.31	0.41
1:C:387:ILE:CG2	1:C:388:GLN:N	2.84	0.41
1:C:1078:ASN:ND2	1:D:1028:ILE:O	2.49	0.41
1:D:1085:SER:OG	1:D:1266:GLU:HG3	2.21	0.41
1:D:51:ASP:OD1	1:D:51:ASP:O	2.39	0.41
1:D:627:LEU:C	1:D:627:LEU:HD13	2.41	0.41
1:D:969:LEU:HA	1:D:1160:PHE:HB3	2.02	0.41
1:A:1256:LYS:NZ	7:A:2174:HOH:O	2.30	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:B:1271:LEU:HA	1:B:1271:LEU:HD23	1.78	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:84:LEU:O	1:B:85:HIS:C	2.59	0.41
1:B:894:TYR:CD1	1:B:894:TYR:N	2.89	0.41
1:D:1203:ALA:O	1:D:1269:THR:HA	2.21	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:A:1055:ALA:HB3	1:A:1066:ILE:HD13	2.02	0.40
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:B:1334:VAL:HG12	1:B:1334:VAL:O	2.21	0.40
1:B:570:VAL:HG11	1:B:582:ARG:NH1	2.36	0.40
1:C:1107:GLU:N	1:C:1108:PRO:HD2	2.36	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: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: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: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:D:147:LEU:O	1:D:148:GLY:C	2.60	0.40
1:D:25:ASP:HA	1:D:26:PRO:HD3	1.91	0.40
1:D:90:THR:CA	7:D:2012:HOH:O	2.68	0.40
1:A: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:A:92:VAL:HG12	1:A:93:GLU:OE1	2.22	0.40
1:B:1203:ALA:O	1:B:1269:THR:HA	2.22	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:72:PHE:HD2	1:B:351:ASN:HB3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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:HG3	1:A:408:GLU:H	1.57	0.40
1:A:764:GLU:HA	1:A:791:ARG:O	2.22	0.40
1:B:1014:PHE:CG	1:B:1019:TYR:HB3	2.57	0.40
1:B:465:GLY:O	1:B:515:ARG:HD2	2.21	0.40
1:B:838:MET:SD	1:B:1228:GLY:N	2.94	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:C:1105:ARG:NH1	1:C:1131:SER:O	2.54	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:CG	1:C:655:GLU:O	2.70	0.40
1:C:973:TRP:O	1:C:977:VAL:HG23	2.21	0.40
1:D:1193:PRO:O	1:D:1197:ILE:HG12	2.22	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:47:CYS:CB	1:D:1229:PRO:HG2	2.52	0.40
1:D:910:LEU:HD23	7:D:2100:HOH:O	2.21	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 ⓘ

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

Some 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
5	MOS	A	3004	4	0,3,3	0.00	-	-		
4	MTE	D	3003	5	21,26,26	1.37	2 (9%)	21,40,40	2.17	6 (28%)
5	MOS	D	3004	4	0,3,3	0.00	-	-		
3	FES	B	3001	1	0,4,4	0.00	-	-		
3	FES	C	3001	1	0,4,4	0.00	-	-		
3	FES	B	3002	1	0,4,4	0.00	-	-		
3	FES	D	3001	1	0,4,4	0.00	-	-		
4	MTE	C	3003	5	21,26,26	1.43	2 (9%)	21,40,40	2.54	7 (33%)
3	FES	A	3002	1	0,4,4	0.00	-	-		
4	MTE	A	3003	5	21,26,26	1.30	2 (9%)	21,40,40	2.18	7 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MOS	B	3004	4	0,3,3	0.00	-	-		
3	FES	A	3001	1	0,4,4	0.00	-	-		
6	FAD	D	3005	-	51,58,58	1.76	6 (11%)	60,89,89	1.89	12 (20%)
6	FAD	A	3005	-	51,58,58	1.76	5 (9%)	60,89,89	1.91	12 (20%)
3	FES	C	3002	1	0,4,4	0.00	-	-		
6	FAD	C	3005	-	51,58,58	1.78	6 (11%)	60,89,89	2.02	11 (18%)
5	MOS	C	3004	4	0,3,3	0.00	-	-		
6	FAD	B	3005	-	51,58,58	1.73	7 (13%)	60,89,89	2.76	14 (23%)
4	MTE	B	3003	5	21,26,26	1.35	2 (9%)	21,40,40	2.15	8 (38%)
3	FES	D	3002	1	0,4,4	0.00	-	-		

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3005	FAD	C4X-C10	9.16	1.48	1.38
6	D	3005	FAD	C4X-C10	9.06	1.47	1.38
6	A	3005	FAD	C4X-C10	9.01	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3005	FAD	C4X-C10	8.52	1.47	1.38
4	C	3003	MTE	C4-C9	4.68	1.47	1.41
4	D	3003	MTE	C4-C9	4.48	1.47	1.41
4	B	3003	MTE	C4-C9	4.20	1.47	1.41
4	A	3003	MTE	C4-C9	4.05	1.47	1.41
6	A	3005	FAD	C4-C4X	3.87	1.48	1.41
6	D	3005	FAD	C4-C4X	3.80	1.47	1.41
6	C	3005	FAD	C4-C4X	3.76	1.47	1.41
4	B	3003	MTE	C9-C10	3.61	1.48	1.41
6	B	3005	FAD	C9A-C5X	3.60	1.49	1.42
6	B	3005	FAD	C4-C4X	3.56	1.47	1.41
6	C	3005	FAD	C9A-C5X	3.56	1.49	1.42
6	D	3005	FAD	C9A-C5X	3.39	1.49	1.42
6	A	3005	FAD	C9A-C5X	3.37	1.49	1.42
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	B	3005	FAD	C9A-N10	2.54	1.41	1.38
6	D	3005	FAD	C9A-N10	2.37	1.41	1.38
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	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	C9A-N10	2.14	1.41	1.38
6	B	3005	FAD	C6-C5X	-2.00	1.38	1.41

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	3005	FAD	C1'-N10-C9A	14.50	129.70	118.29
6	C	3005	FAD	C4-N3-C2	8.43	122.26	115.14
6	B	3005	FAD	C4-N3-C2	8.36	122.20	115.14
6	D	3005	FAD	C4-N3-C2	8.11	121.99	115.14
6	A	3005	FAD	C4-N3-C2	8.09	121.97	115.14
4	C	3003	MTE	O3'-C7-C6	-7.24	104.14	108.96
6	C	3005	FAD	C1'-N10-C9A	6.83	123.67	118.29
6	B	3005	FAD	C1'-N10-C10	-6.07	112.97	118.41
6	A	3005	FAD	C1'-N10-C9A	5.21	122.39	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3005	FAD	C4-C4X-C10	-5.08	116.59	119.95
6	B	3005	FAD	C4-C4X-C10	-5.07	116.59	119.95
6	A	3005	FAD	C4-C4X-C10	-4.39	117.05	119.95
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
6	D	3005	FAD	C4X-N5-C5X	4.30	121.07	116.77
6	D	3005	FAD	C4-C4X-C10	-4.26	117.13	119.95
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
6	D	3005	FAD	C1'-N10-C9A	4.05	121.48	118.29
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	C4-N3-C2	3.75	121.88	115.93
6	A	3005	FAD	C4X-N5-C5X	3.72	120.49	116.77
6	A	3005	FAD	C4X-C4-N3	-3.70	118.37	123.43
4	D	3003	MTE	C4-N3-C2	3.68	121.78	115.93
6	C	3005	FAD	C4X-C4-N3	-3.68	118.40	123.43
4	A	3003	MTE	C10-N8-C7	-3.67	116.48	123.67
6	B	3005	FAD	C4X-C4-N3	-3.66	118.43	123.43
4	D	3003	MTE	O3'-C7-C6	-3.66	106.52	108.96
4	C	3003	MTE	C4-N3-C2	3.65	121.72	115.93
6	D	3005	FAD	C4X-C4-N3	-3.64	118.45	123.43
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	C9A-N10-C10	-3.53	117.28	121.91
6	B	3005	FAD	N3A-C2A-N1A	-3.47	123.25	128.68
6	C	3005	FAD	C4X-N5-C5X	3.40	120.17	116.77
6	B	3005	FAD	C4X-N5-C5X	3.31	120.08	116.77
4	B	3003	MTE	C4-N3-C2	3.30	121.17	115.93
6	D	3005	FAD	N3A-C2A-N1A	-3.26	123.59	128.68
6	B	3005	FAD	C4-C4X-N5	3.23	122.29	118.60
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
6	C	3005	FAD	C9A-N10-C10	-3.14	117.80	121.91
4	B	3003	MTE	C4-C9-C10	3.09	117.31	114.57
6	A	3005	FAD	N3A-C2A-N1A	-3.05	123.91	128.68
6	A	3005	FAD	C9A-N10-C10	-3.02	117.95	121.91
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	C9A-N10-C10	-2.90	118.11	121.91
6	C	3005	FAD	C4-C4X-N5	2.88	121.89	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3005	FAD	P-O3P-PA	-2.86	123.02	132.83
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
6	A	3005	FAD	C4-C4X-N5	2.69	121.67	118.60
4	C	3003	MTE	C4-C9-C10	2.69	116.96	114.57
6	D	3005	FAD	C4-C4X-N5	2.68	121.67	118.60
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	A	3005	FAD	C3B-C2B-C1B	2.58	104.86	100.98
6	D	3005	FAD	C3B-C2B-C1B	2.56	104.83	100.98
4	B	3003	MTE	O3'-C7-N8	2.48	111.11	108.57
6	B	3005	FAD	C4A-C5A-N7A	-2.43	106.87	109.40
4	D	3003	MTE	C4-C9-C10	2.36	116.66	114.57
4	C	3003	MTE	O2P-P-O4'	-2.26	100.71	106.73
6	D	3005	FAD	C1'-N10-C10	2.21	120.39	118.41
6	C	3005	FAD	C5X-C9A-N10	2.20	119.31	117.72
6	A	3005	FAD	C5X-C9A-N10	2.17	119.29	117.72
6	B	3005	FAD	C3B-C2B-C1B	2.14	104.20	100.98
4	A	3003	MTE	C4-C9-C10	2.13	116.46	114.57
4	B	3003	MTE	O3P-P-O2P	2.10	115.65	107.64
6	B	3005	FAD	O2'-C2'-C1'	2.08	114.61	109.59
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	C	3005	FAD	C5B-O5B-PA-O1A
6	C	3005	FAD	C5B-O5B-PA-O3P
6	C	3005	FAD	C2'-C1'-N10-C9A
6	C	3005	FAD	C2'-C1'-N10-C10
6	C	3005	FAD	N10-C1'-C2'-O2'
6	C	3005	FAD	N10-C1'-C2'-C3'

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Mol	Chain	Res	Type	Atoms
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	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	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'

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Mol	Chain	Res	Type	Atoms
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'

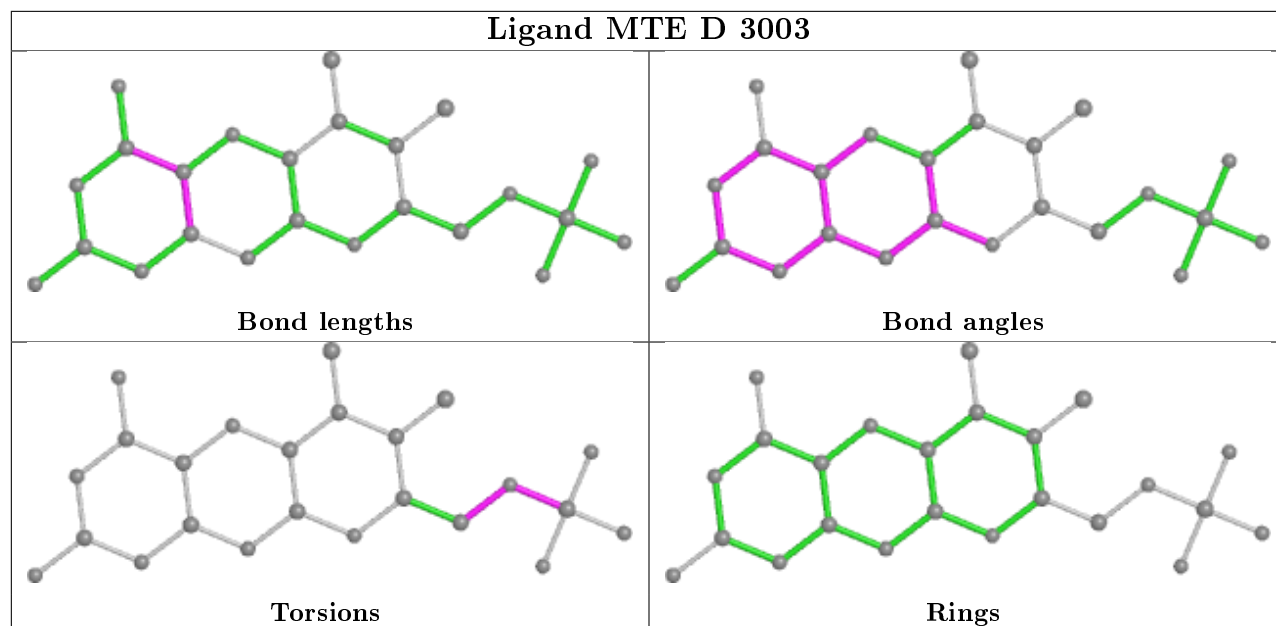
There are no ring outliers.

16 monomers are involved in 82 short contacts:

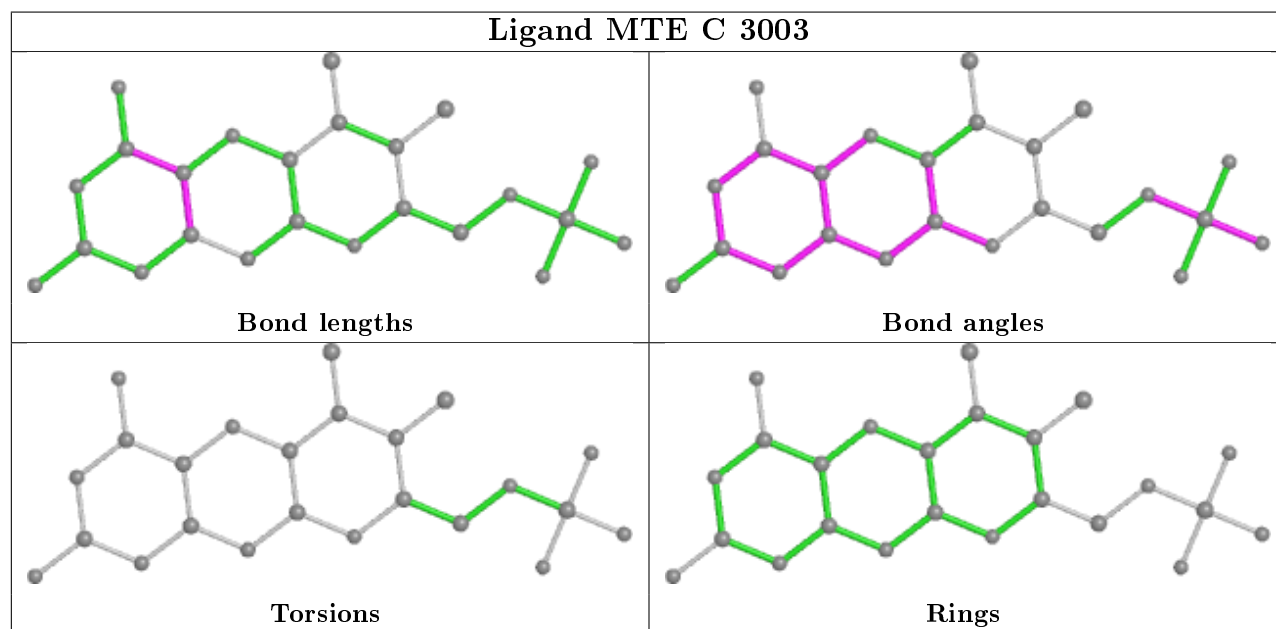
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	3004	MOS	2	0
4	D	3003	MTE	3	0
5	D	3004	MOS	2	0
3	B	3002	FES	1	0
4	C	3003	MTE	3	0
3	A	3002	FES	1	0
4	A	3003	MTE	4	0
5	B	3004	MOS	2	0
6	D	3005	FAD	15	0
6	A	3005	FAD	8	0
3	C	3002	FES	1	0
6	C	3005	FAD	21	0
5	C	3004	MOS	2	0
6	B	3005	FAD	14	0
4	B	3003	MTE	1	0
3	D	3002	FES	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

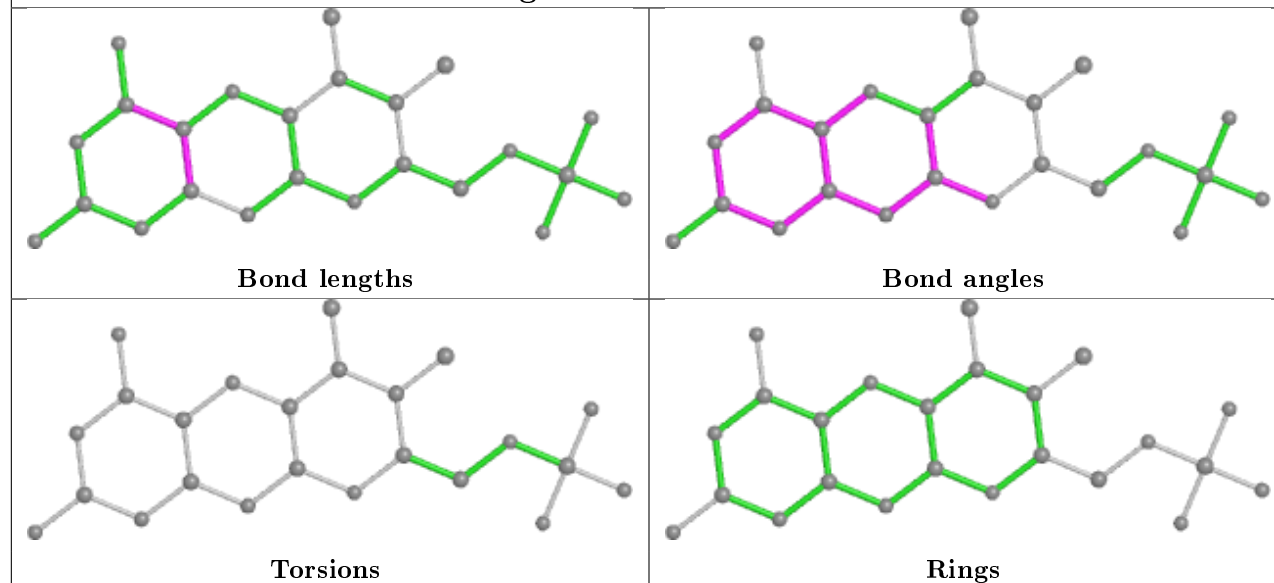
Ligand MTE D 3003



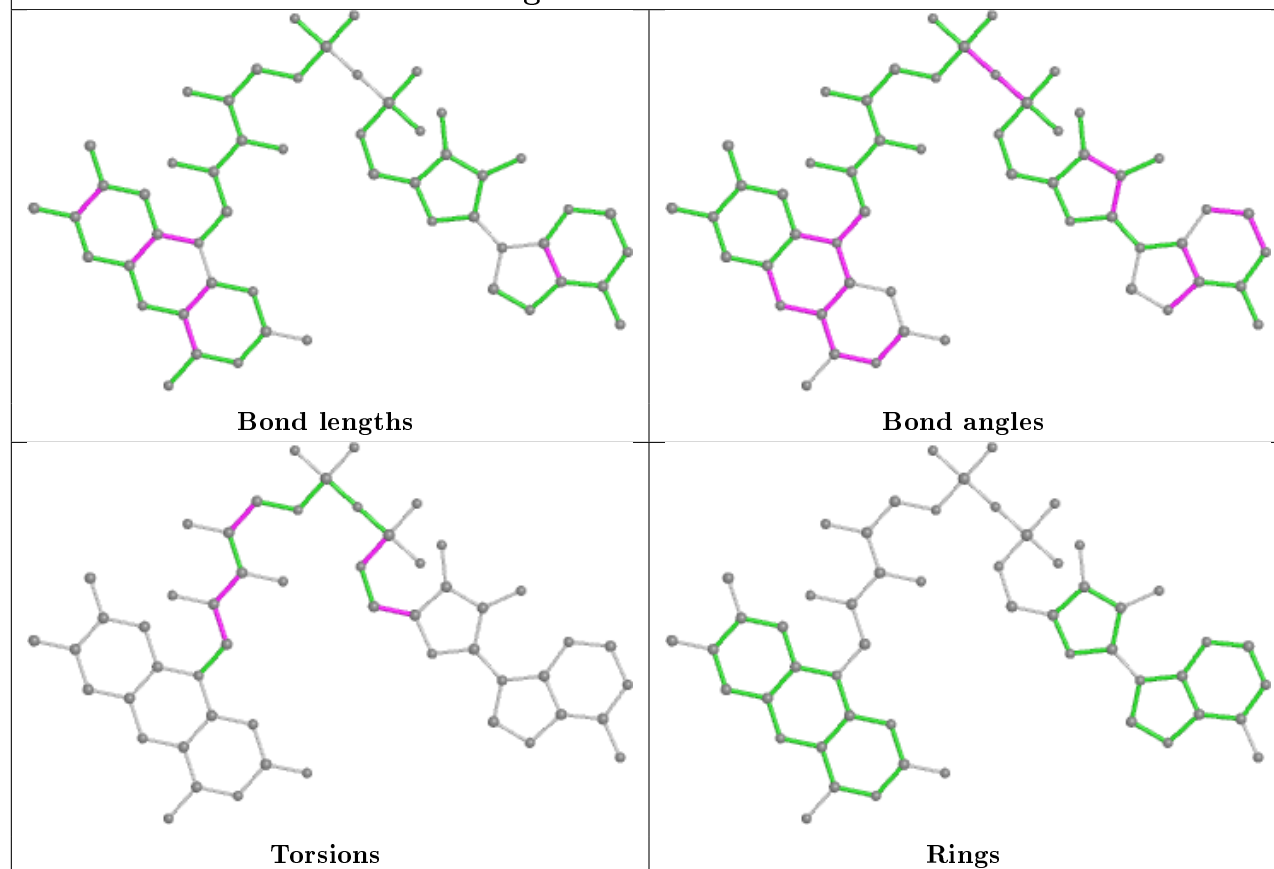
Ligand MTE C 3003

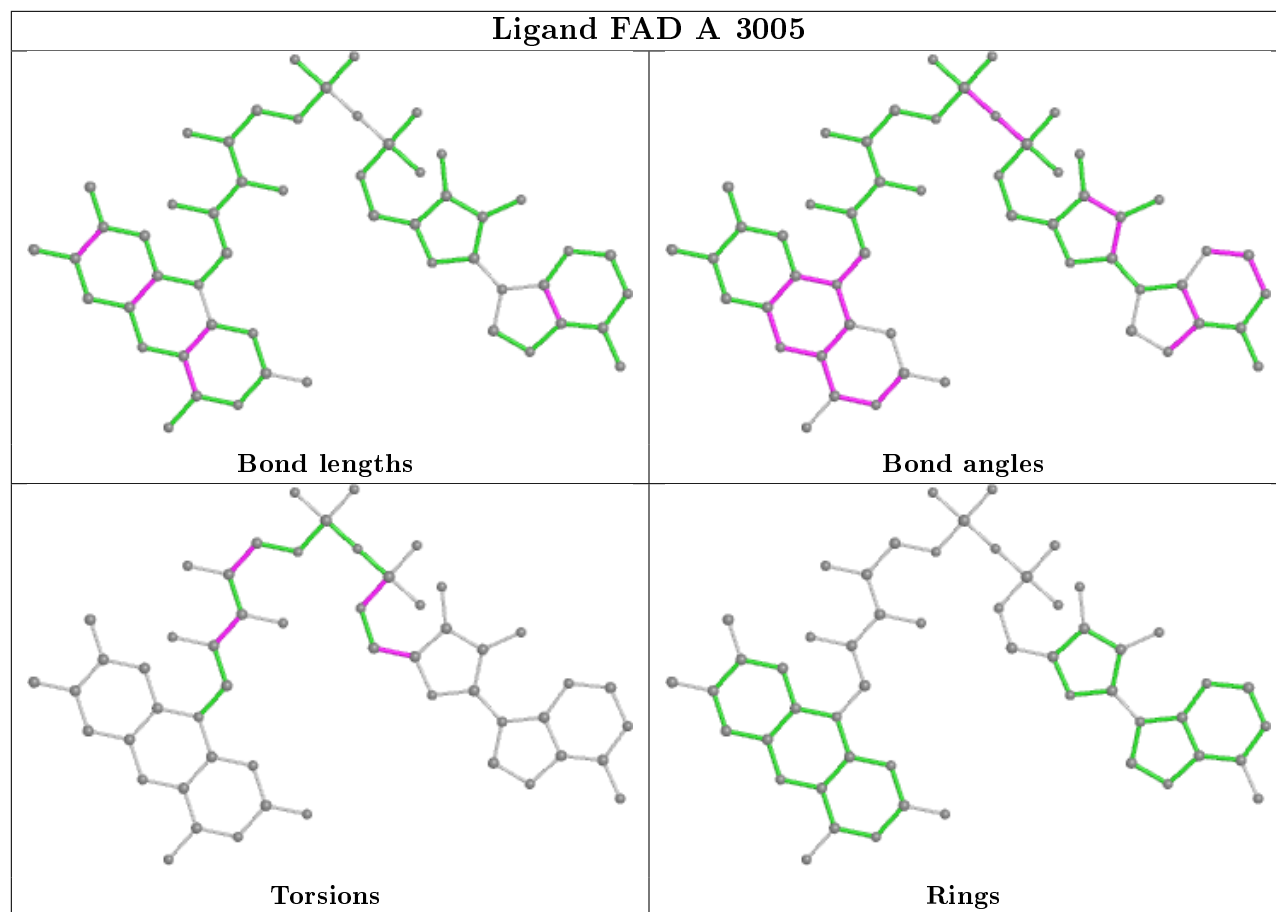


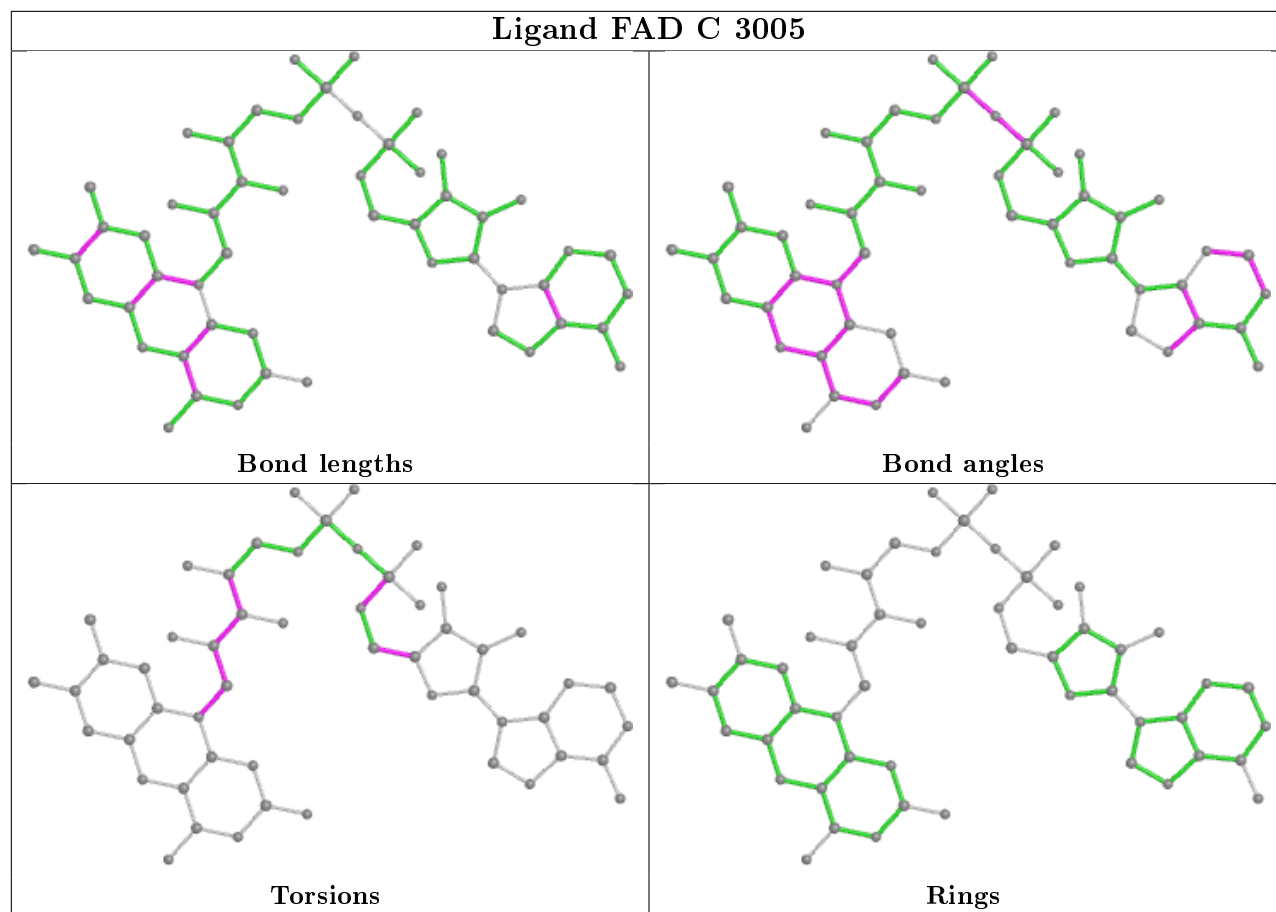
Ligand MTE A 3003

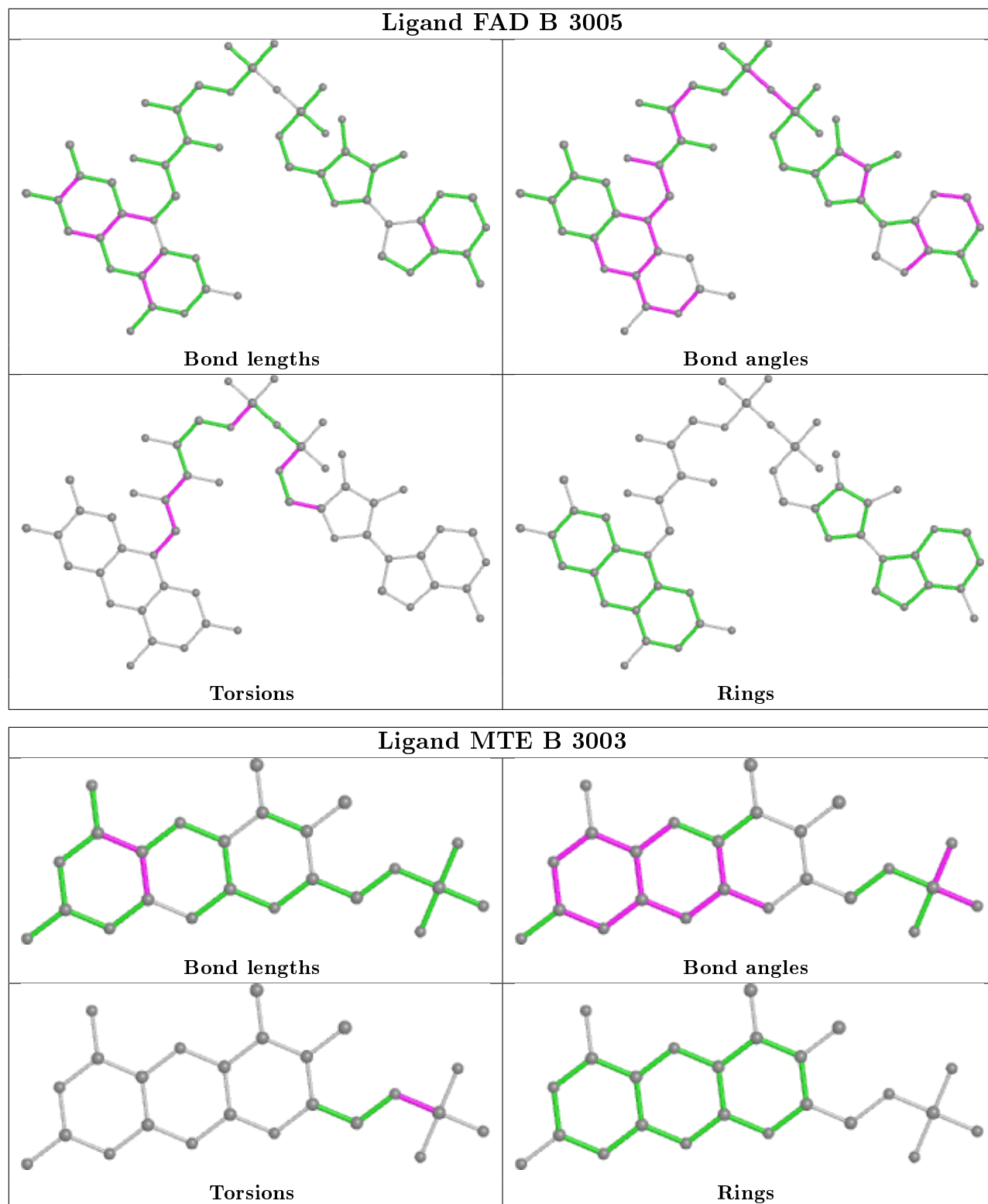


Ligand FAD D 3005









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

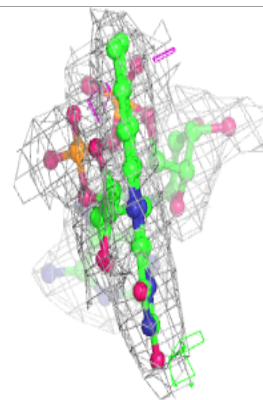
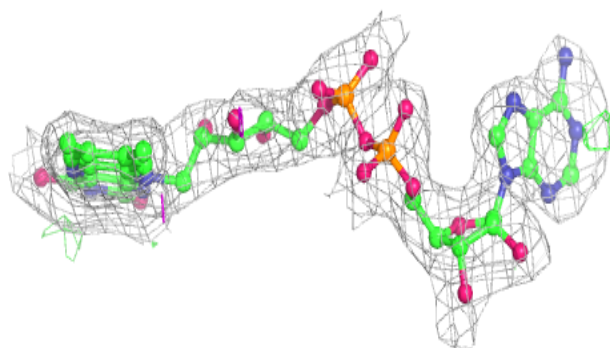
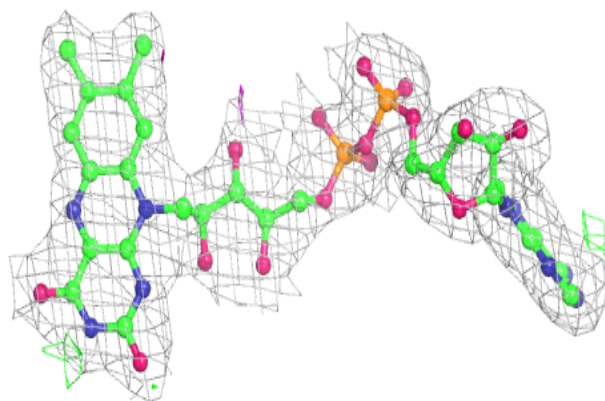
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

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

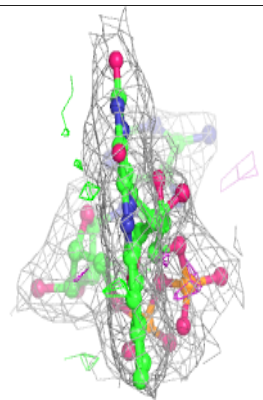
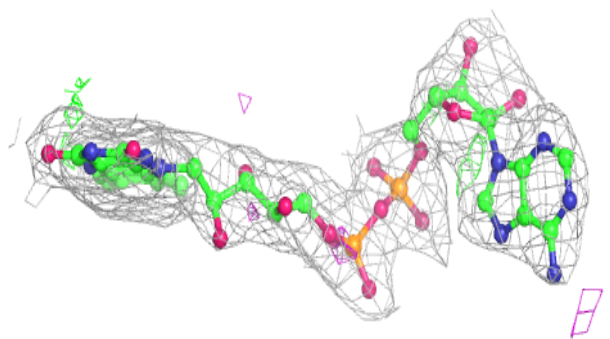
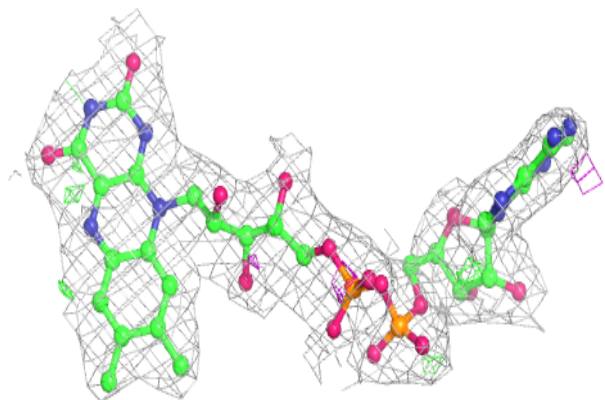
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD 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)

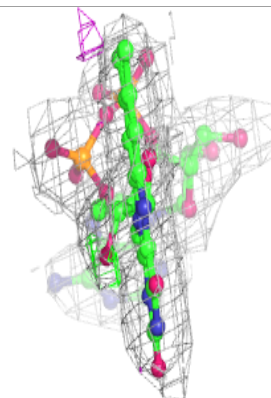
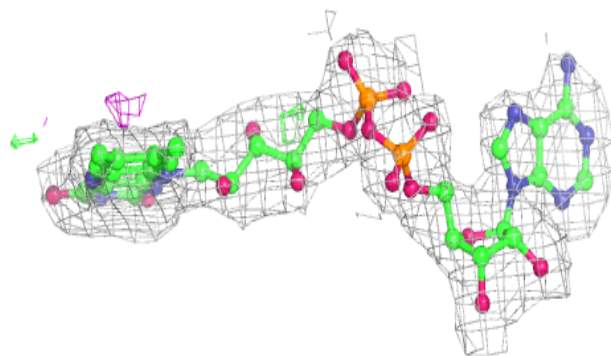
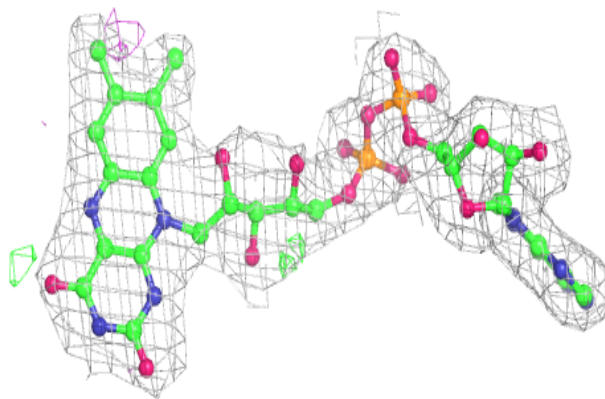
**Electron density around FAD C 3005:**

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

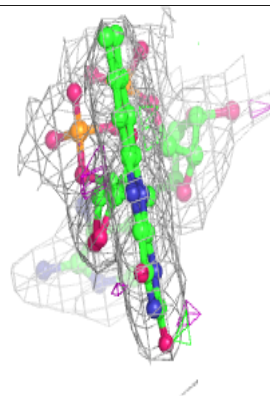
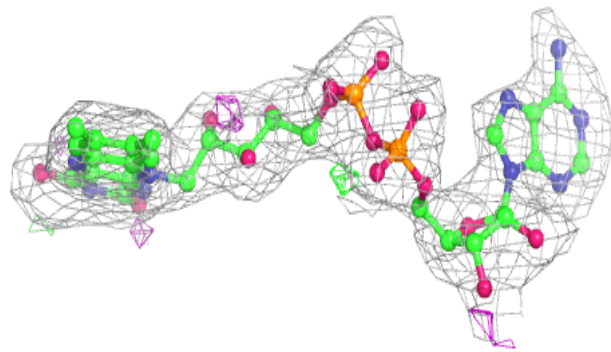
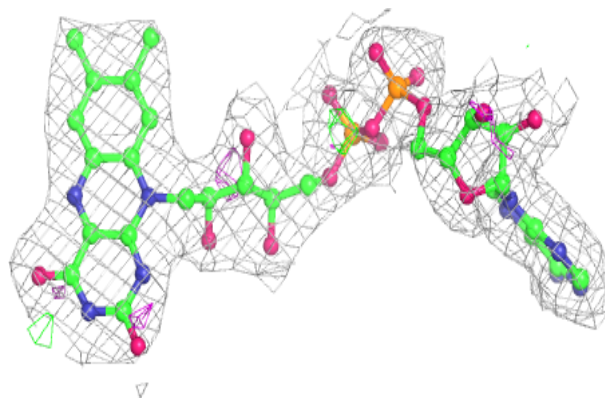


Electron density around FAD B 3005:

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

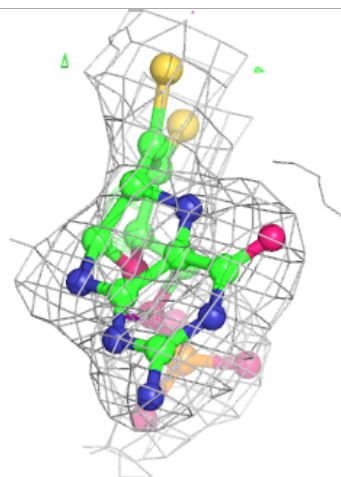
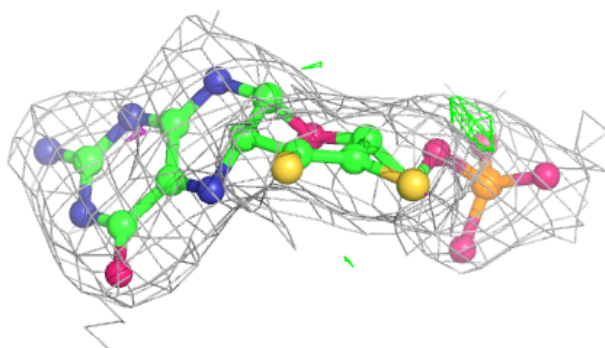
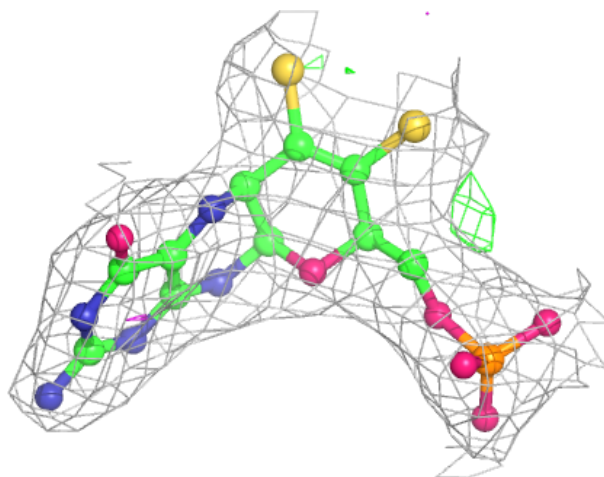
**Electron density around FAD A 3005:**

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



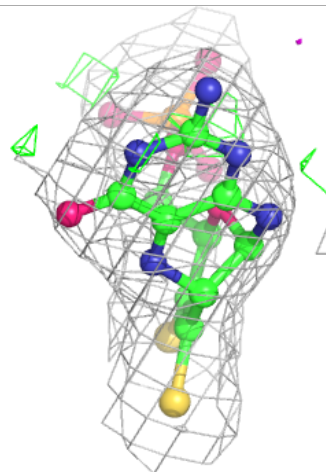
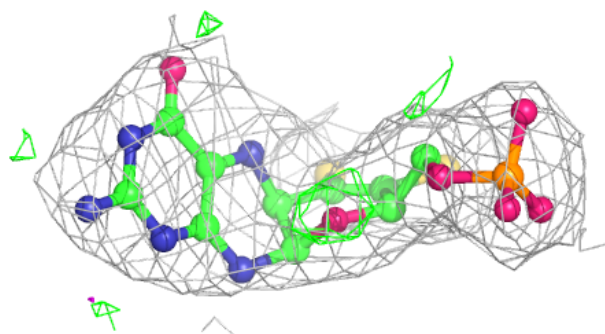
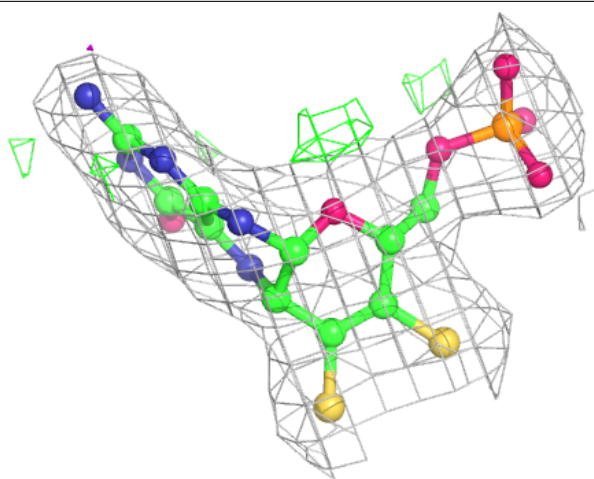
Electron density around MTE B 3003:

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



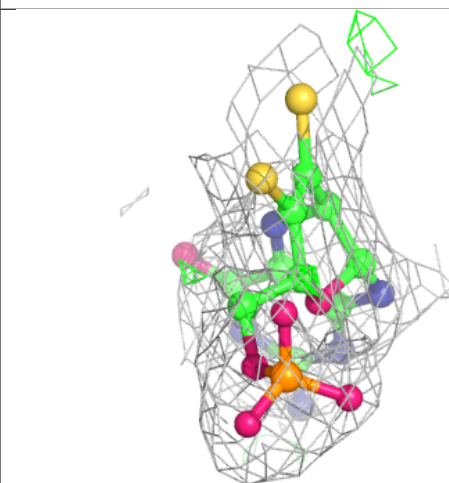
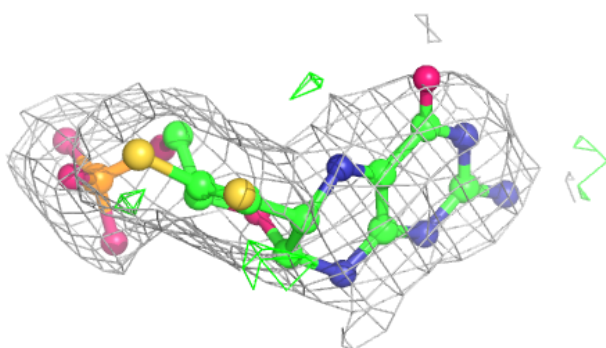
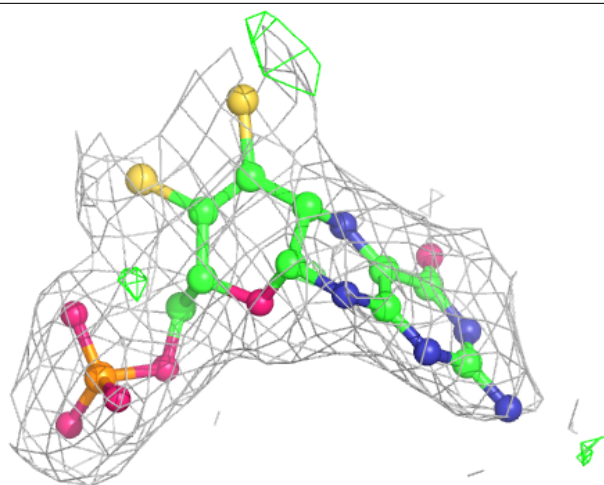
Electron density around MTE A 3003:

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



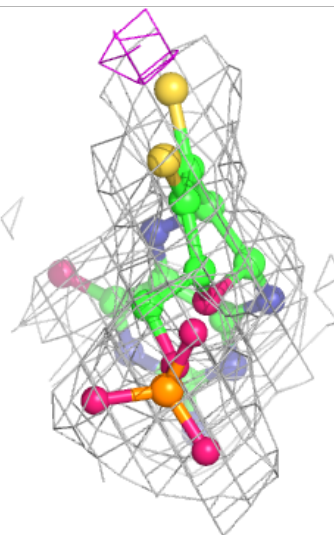
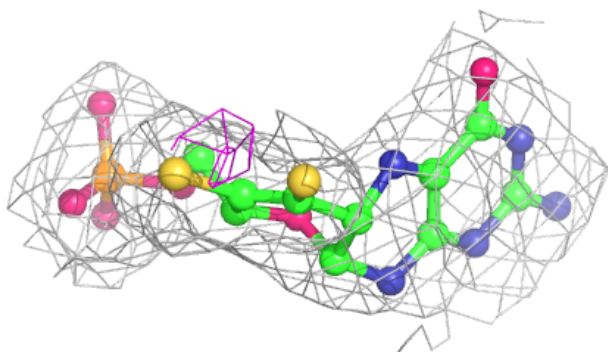
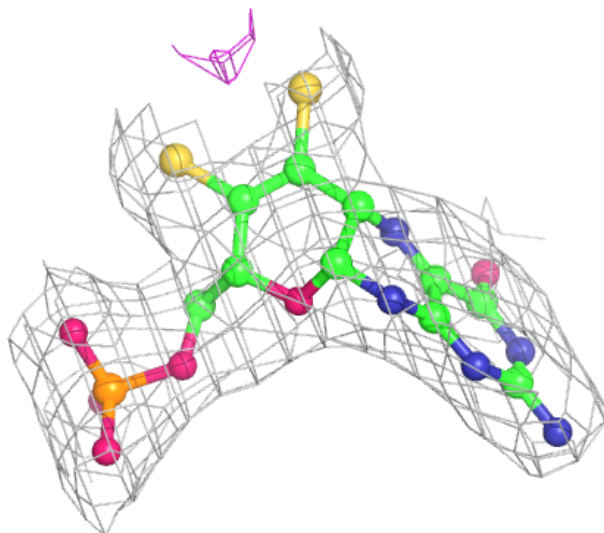
Electron density around MTE D 3003:

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



Electron density around MTE C 3003:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.