



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:43 PM GMT

PDB ID : 3UKP
Title : Crystal structure of R327A UDP-galactopyranose mutase from *Aspergillus fumigatus* in complex with UDPgalp
Authors : Van Straaten, K.E.; Sanders, D.A.R.
Deposited on : 2011-11-09
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

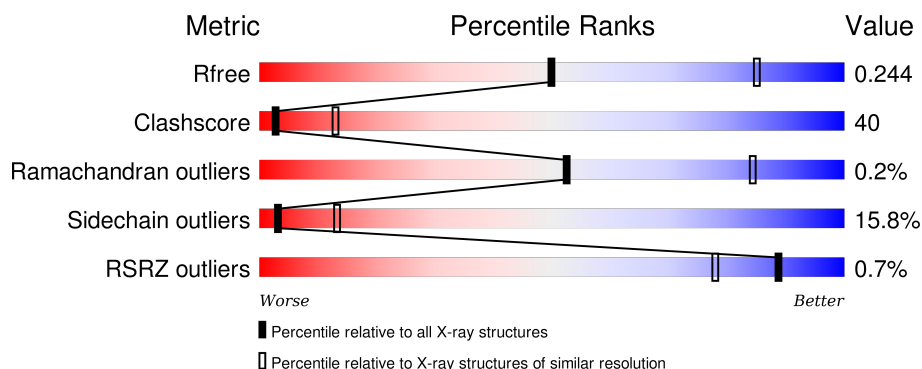
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



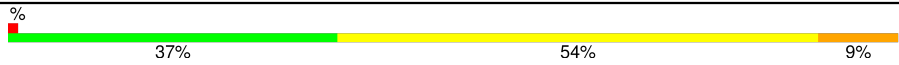
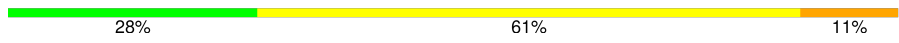

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	509	<div> <div></div> <div> <div></div> <div>50%</div> <div>43%</div> <div>7%</div> </div> </div>
1	B	509	<div> <div></div> <div> <div></div> <div>48%</div> <div>44%</div> <div>8%</div> </div> </div>
1	C	509	<div> <div></div> <div> <div></div> <div>49%</div> <div>45%</div> <div>6%</div> </div> </div>
1	D	509	<div> <div></div> <div> <div></div> <div>50%</div> <div>43%</div> <div>7%</div> </div> </div>
1	E	509	<div> <div></div> <div> <div></div> <div>37%</div> <div>55%</div> <div>9%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	509	
1	G	509	
1	H	509	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FAD	A	601	X	-	-	-
2	FAD	D	601	-	-	X	-
2	FAD	F	601	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 32560 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 UDP-galactopyranose mutase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	B	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	C	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	D	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	E	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	F	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	G	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			
1	H	509	Total	C	N	O	S	0	0	0
			3990	2531	683	755	21			

There are 8 discrepancies between the modelled and reference sequences:

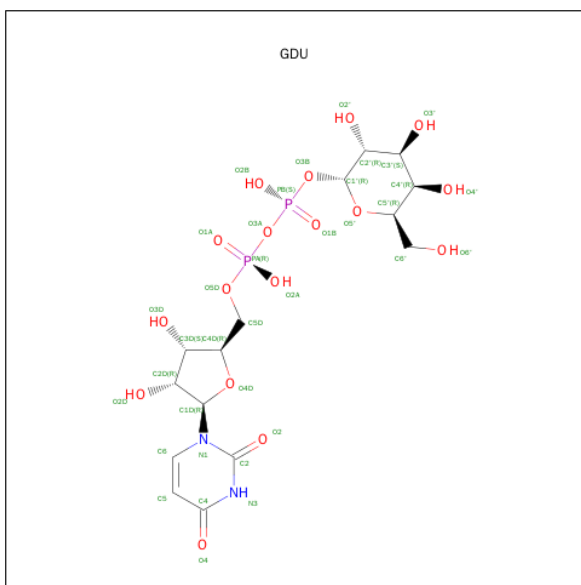
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
B	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
C	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
D	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
E	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
F	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
G	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2
H	327	ALA	ARG	ENGINEERED MUTATION	UNP Q4W1X2

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



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

- Molecule 3 is SUGAR (GALACTOSE-URIDINE-5'-DIPHOSPHATE) (three-letter code: GDU) (formula: C₁₅H₂₄N₂O₁₇P₂).

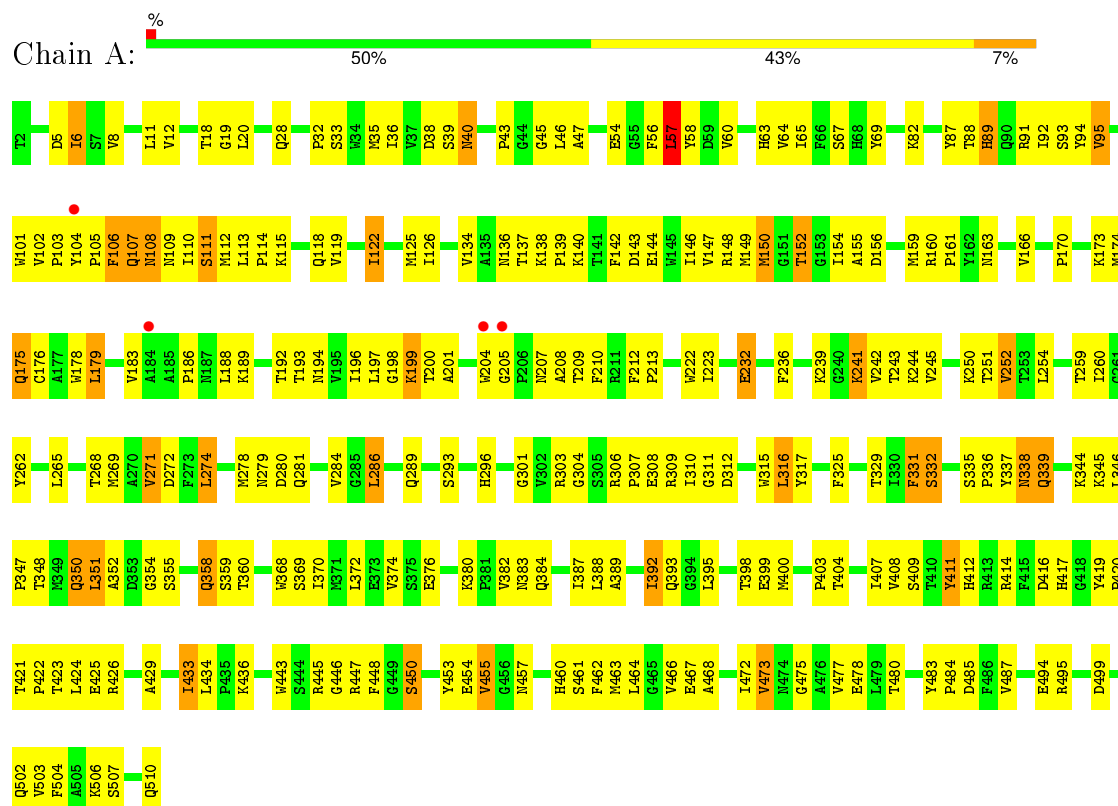


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	B	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	D	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	C	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	E	1	Total 36	C 15	N 2	O 17	P 2	0	0
3	F	1	Total 36	C 15	N 2	O 17	P 2	0	0

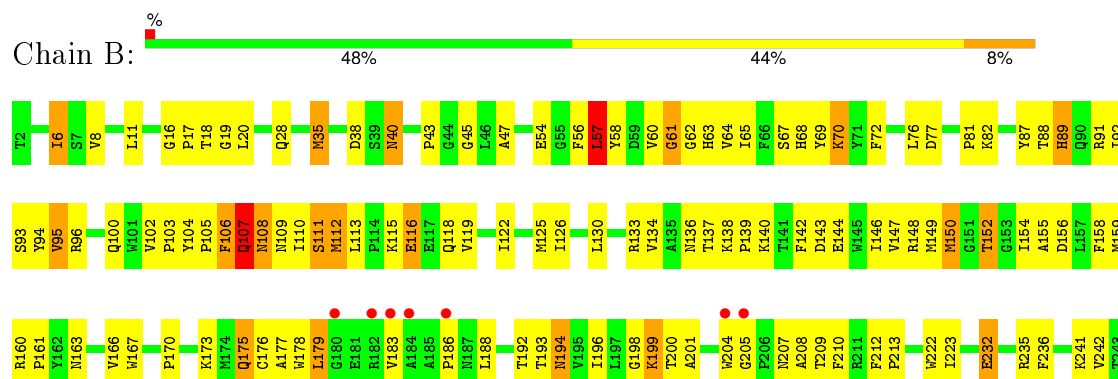
3 Residue-property plots

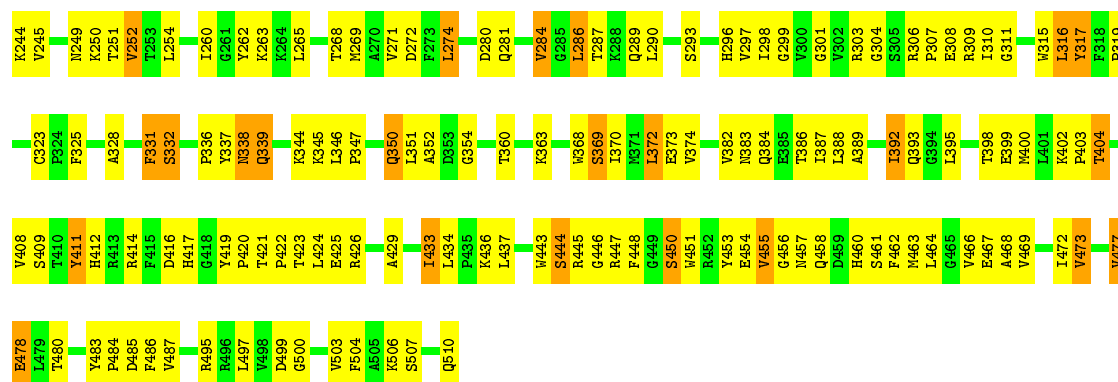
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: UDP-galactopyranose mutase

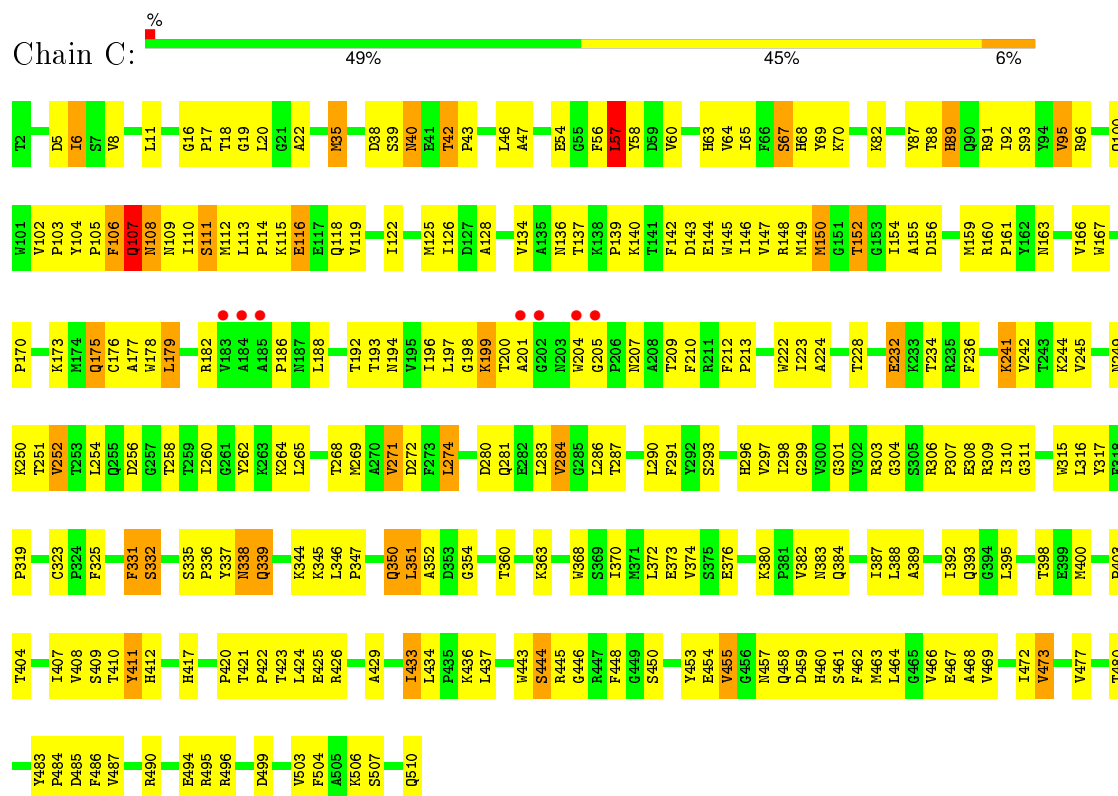


• Molecule 1: UDP-galactopyranose mutase

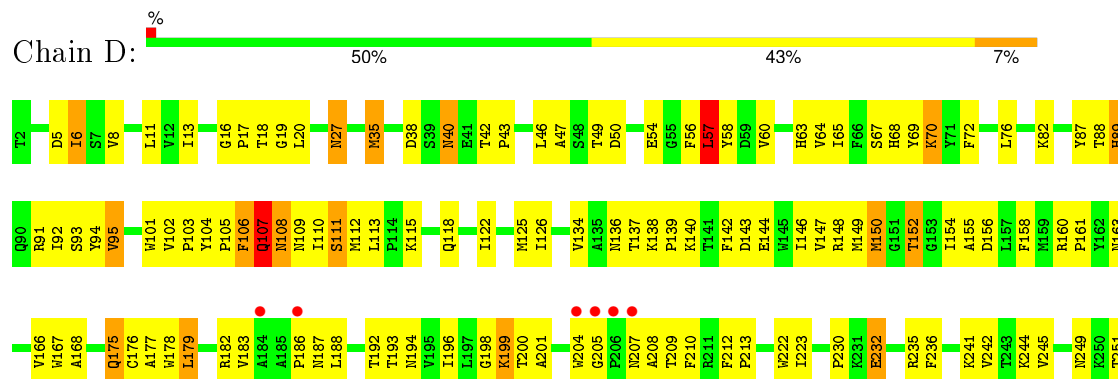


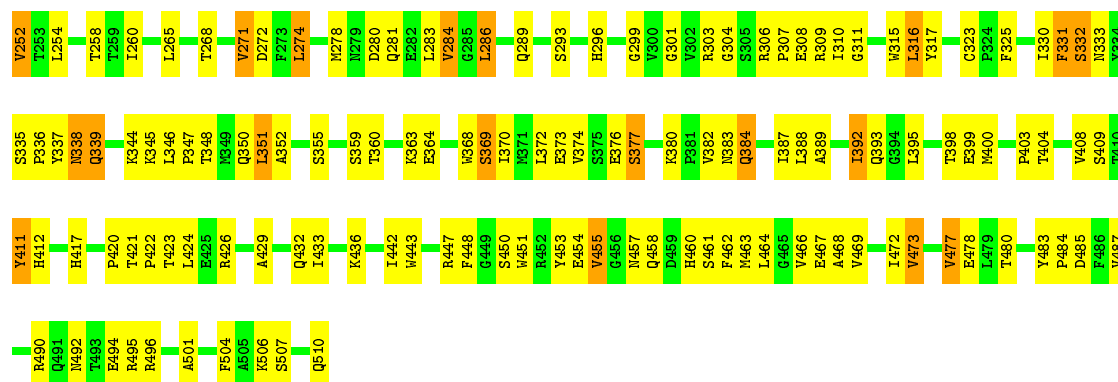


• Molecule 1: UDP-galactopyranose mutase



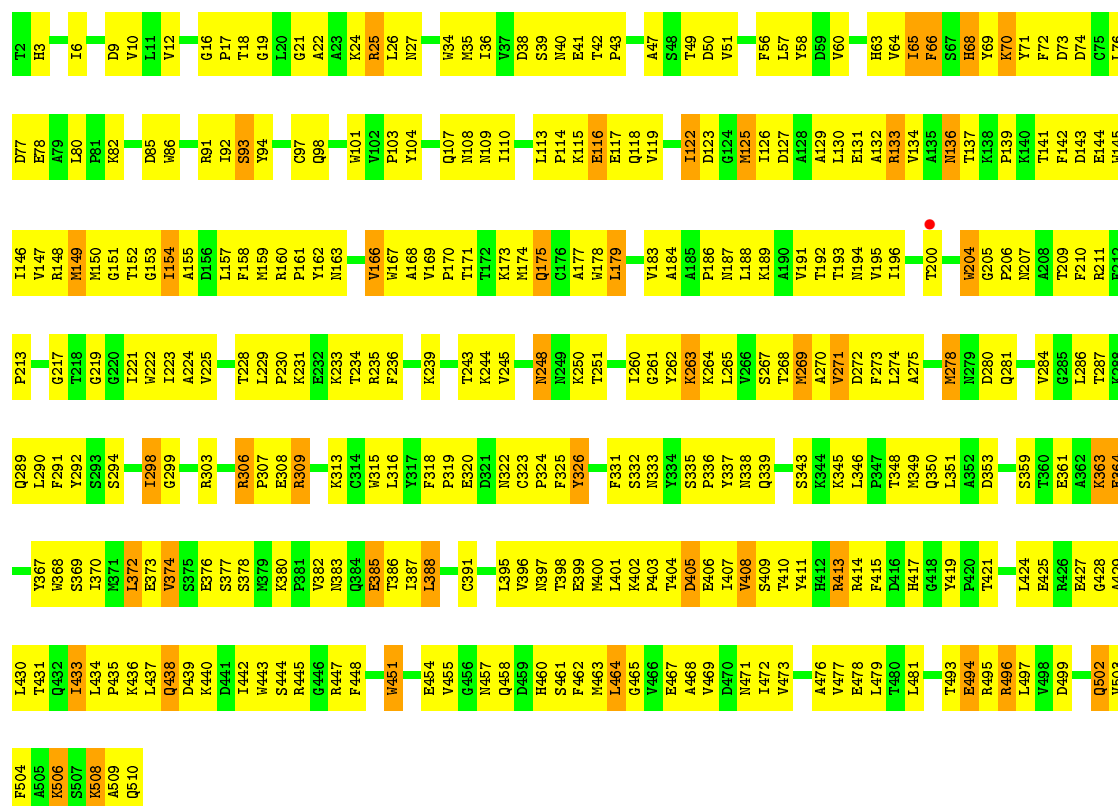
• Molecule 1: UDP-galactopyranose mutase





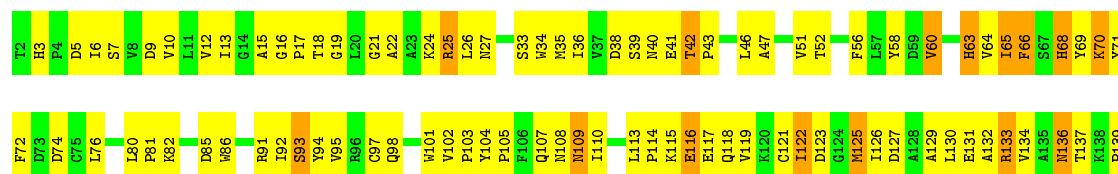
• Molecule 1: UDP-galactopyranose mutase

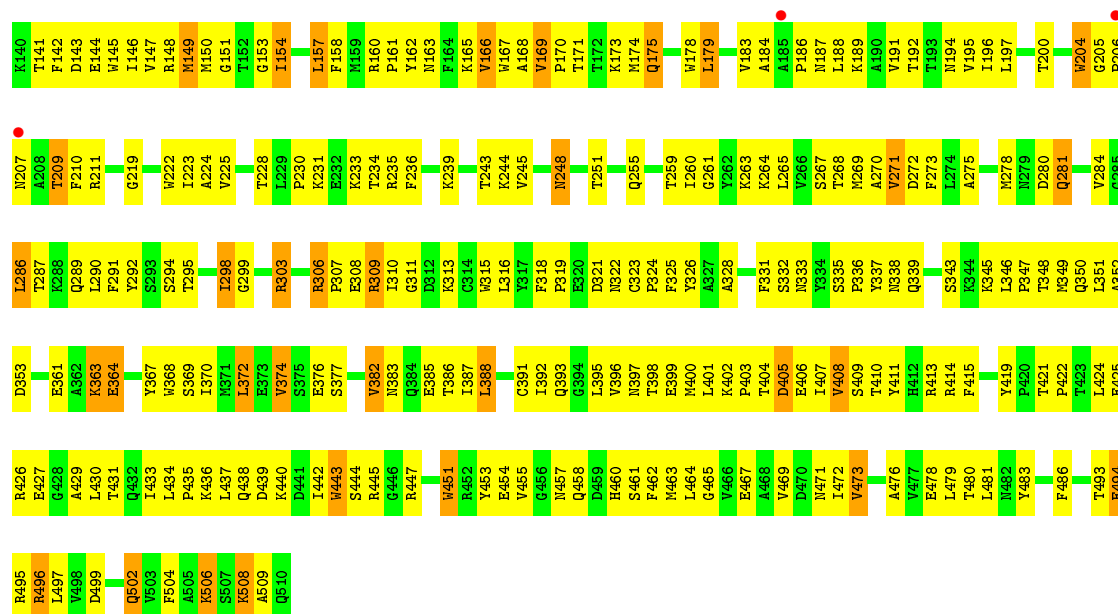
Chain E: 37% 55% 9%



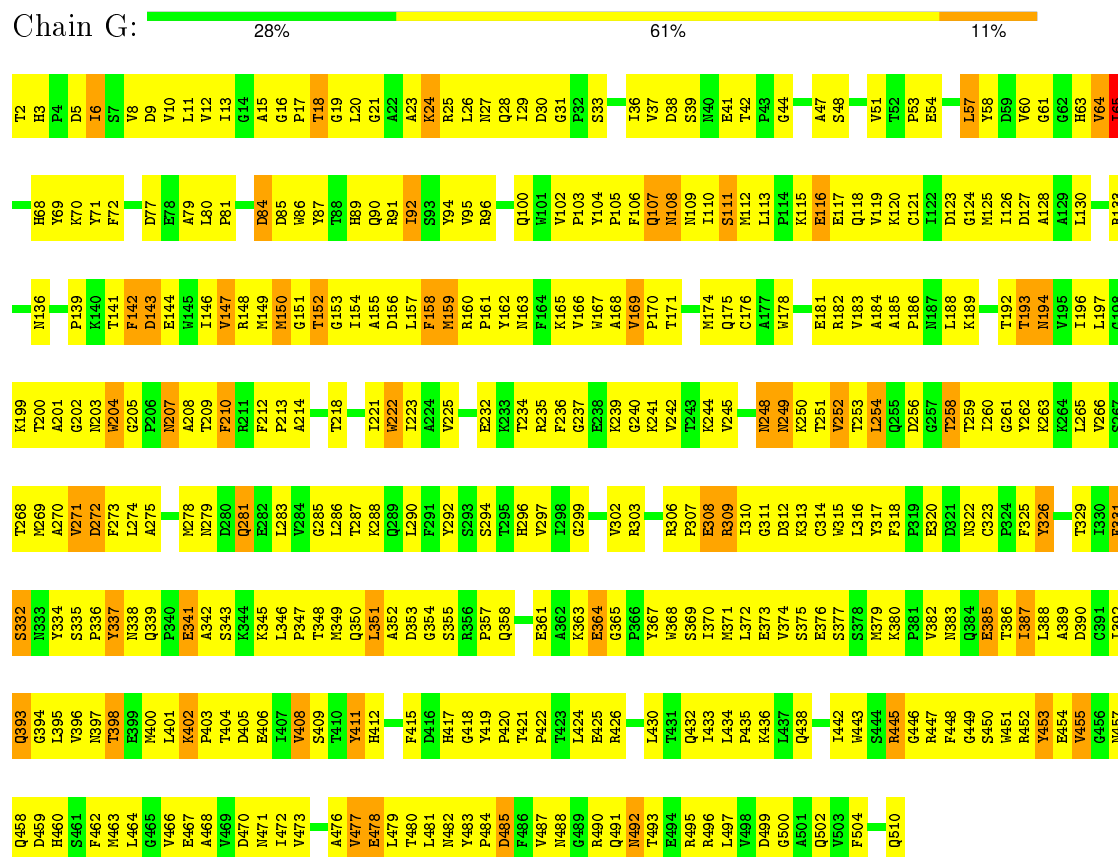
• Molecule 1: UDP-galactopyranose mutase

Chain F: 37% 54% 9%

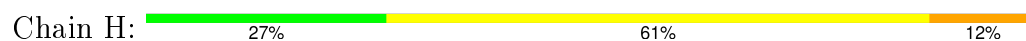




• Molecule 1: UDP-galactopyranose mutase



• Molecule 1: UDP-galactopyranose mutase



Q458	L395	Y334	T268	K199	R133	S67	T2
D459	V396	S336	T269	T200	V134	H68	H3
H460	N397	P336	A270	A201	P139	Y69	P4
S461	T398	T337	V271	G202	K140	K70	D5
F462	E399	N338	D272	N203	T141	S7	I6
H463	M400	D339	T273	G205	F142	Y71	S7
L464	L401	P340	L274	F206	D143	V72	V8
G465	K402	E341	A275	E144	E145	D77	D9
V466	P403	A342	E276	A207	H146	E78	V10
E467	T404	S343	A277	A208	W147	A79	L11
A468	D405	S344	M278	T209	R148	L80	V12
Y469	E406	K345	D280	F210	M149	P81	I13
D470	L407	I346	Q281	F212	M150	K82	G14
N471	V408	P347	Q282	F213	D84	E83	A15
L472	S409	T348	E282	A214	D85	G16	G16
V473	T410	P349	L283	T218	W86	P17	P17
A476	Y411	Q350	V284	G153	Y87	L20	L20
V477	H412	L351	G285	G219	T88	G21	G21
E478	F415	A352	L286	G220	H89	A22	A22
L479	D416	D353	T287	I221	Q90	A23	A23
T480	H417	G354	K288	W222	R91	K24	K24
L481	G418	S355	Q289	I223	F158	R25	R25
N482	G418	K356	L290	A224	M159	S93	L26
Y483	Y419	P357	F291	V225	R160	Y94	Y94
P484	P420	O358	Y292	A226	P161	V95	Q28
D485	T421	S359	S293	L229	Y162	R96	L29
F486	P422	T360	S294	M163	N163	D30	D30
Y487	T423	E361	T295	T234	F164	G31	G31
N488	L424	A362	H296	R235	K165	P32	P32
G489	E425	K363	V297	F236	V166	S33	S33
R490	R426	E364	L298	G237	W167	W34	W34
Q491	L430	P366	V302	E238	V169	P103	P103
N492	T431	Y367	R303	K241	T171	F104	F104
T493	Q432	W368	V307	V242	M174	P105	P105
E494	I433	S369	E308	T243	Q175	F106	F106
R495	L434	I370	R309	K244	C176	V107	V107
R496	P435	N371	I310	V245	A177	D108	D108
L497	K436	L372	G311	N249	W178	S39	S39
V498	Q438	E373	D312	K250	E181	N109	N109
D499	Q438	S375	K313	T251	E182	I110	I110
G500	D439	E376	W315	V252	V183	S111	T32
A501	K440	S377	L316	T253	A184	M112	P43
Q502	D441	S377	Y317	L254	M187	L113	Q44
F503	I442	S378	F318	D255	K188	P114	P114
F504	W443	P379	N322	G257	K189	K115	A47
S507	S444	V382	C323	T258	A190	E116	S48
Q510	G446	N383	P324	T259	V191	E117	S48
	R447	Q384	F325	I260	T193	Q118	V51
	F448	E386	Y326	G261	N194	V119	V51
	G449	T386	C391	Y262	V195	K120	B54
	S450	I387	I392	K263	A128	C121	L57
	W451	L388	S332	K264	V196	I122	L57
	A452	A389	F333	N333	L197	D123	Y58
	Y453	D390	G394		G198	M125	D59
	E454	C391				I126	V60
	V455	I392				D127	G61
	G456	Q393				A129	G62
	N457	G394				V64	H63
						L130	V64
						P66	P66

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.60Å 175.71Å 135.35Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	34.77 – 3.10 34.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.3 (34.77-3.10) 96.2 (34.77-3.10)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	0.24	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.7.1_743)	Depositor
R, R_{free}	0.202 , 0.260 0.201 , 0.244	Depositor DCC
R_{free} test set	5331 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.479 for H,-K,-L 0.000 for l,k,-h 0.327 for h,-k,-l 0.000 for l,-k,h	Xtriage
Reported twinning fraction	0.479 for H,-K,-L	Depositor
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 105627 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	32560	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.04 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6278e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GDU, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.30	0/4089	0.55	1/5558 (0.0%)
1	B	0.30	0/4089	0.55	1/5558 (0.0%)
1	C	0.30	0/4089	0.55	1/5558 (0.0%)
1	D	0.30	0/4089	0.55	1/5558 (0.0%)
1	E	0.32	0/4089	0.57	0/5558
1	F	0.32	0/4089	0.58	0/5558
1	G	0.32	0/4089	0.61	2/5558 (0.0%)
1	H	0.31	0/4089	0.59	1/5558 (0.0%)
All	All	0.31	0/32712	0.57	7/44464 (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	G	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	LEU	CA-CB-CG	6.50	130.25	115.30
1	G	205	GLY	O-C-N	-6.40	108.95	121.10
1	B	57	LEU	CA-CB-CG	6.33	129.85	115.30
1	H	205	GLY	N-CA-C	-5.37	99.66	113.10
1	A	57	LEU	CA-CB-CG	5.24	127.35	115.30
1	G	205	GLY	CA-C-N	5.20	131.67	117.10
1	D	57	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	65	ILE	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	3990	0	3906	244	0
1	B	3990	0	3906	267	0
1	C	3990	0	3906	265	0
1	D	3990	0	3906	233	0
1	E	3990	0	3906	386	0
1	F	3990	0	3906	359	0
1	G	3990	0	3906	446	0
1	H	3990	0	3906	430	0
2	A	53	0	29	10	0
2	B	53	0	30	14	0
2	C	53	0	30	12	0
2	D	53	0	30	22	0
2	E	53	0	30	20	0
2	F	53	0	29	14	0
2	G	53	0	29	13	0
2	H	53	0	30	10	0
3	A	36	0	22	9	0
3	B	36	0	22	15	0
3	C	36	0	22	9	0
3	D	36	0	22	4	0
3	E	36	0	22	14	0
3	F	36	0	22	8	0
All	All	32560	0	31617	2587	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 40.

All (2587) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LYS:HG3	1:E:496:ARG:HH22	0.96	1.10
1:F:70:LYS:HG3	1:F:496:ARG:HH22	1.12	1.10
1:F:461:SER:HA	1:F:464:LEU:HD12	1.37	1.06
1:D:303:ARG:NH2	1:D:346:LEU:O	1.90	1.05
1:E:461:SER:HA	1:E:464:LEU:HD12	1.38	1.05
1:B:332:SER:HA	1:B:339:GLN:HE21	1.20	1.04
1:E:133:ARG:HH11	1:E:133:ARG:HG3	1.24	1.02
1:F:16:GLY:HA3	2:F:601:FAD:O1P	1.59	1.02
1:B:62:GLY:O	3:B:602:GDU:O4'	1.76	1.01
1:B:183:VAL:HG22	3:B:602:GDU:H1D	1.36	1.01
1:A:303:ARG:NH2	1:A:346:LEU:O	1.95	1.00
1:H:149:MET:SD	1:H:184:ALA:HA	2.01	1.00
1:G:17:PRO:HD2	2:G:601:FAD:O1P	1.60	0.99
1:D:332:SER:HA	1:D:339:GLN:HE21	1.24	0.99
1:A:104:TYR:HE1	3:A:602:GDU:H5	1.26	0.98
1:A:183:VAL:HG13	3:A:602:GDU:O2	1.65	0.96
1:A:104:TYR:CE1	3:A:602:GDU:H5	2.00	0.96
1:G:115:LYS:HA	1:G:118:GLN:HG3	1.47	0.95
1:C:332:SER:HA	1:C:339:GLN:HE21	1.30	0.95
1:G:18:THR:HG22	1:G:268:THR:HG21	1.49	0.94
1:F:154:ILE:HD13	1:F:154:ILE:H	1.31	0.94
1:G:197:LEU:C	1:G:199:LYS:H	1.70	0.94
1:G:292:TYR:HB2	1:G:419:TYR:O	1.67	0.94
1:E:70:LYS:HG3	1:E:496:ARG:NH2	1.81	0.94
1:A:244:LYS:HB2	1:F:255:GLN:HE21	1.30	0.94
1:H:292:TYR:HB2	1:H:419:TYR:O	1.69	0.93
1:A:332:SER:HA	1:A:339:GLN:HE21	1.34	0.93
1:F:445:ARG:HB3	1:F:464:LEU:HB3	1.51	0.92
1:G:47:ALA:HB3	1:G:222:TRP:HE1	1.34	0.92
1:H:150:MET:HG3	1:H:154:ILE:HB	1.51	0.92
1:F:133:ARG:HH11	1:F:133:ARG:HG3	1.31	0.92
1:F:467:GLU:HG3	1:F:495:ARG:HH12	1.36	0.91
1:B:183:VAL:HG13	3:B:602:GDU:C2	2.01	0.91
1:F:9:ASP:HA	1:F:263:LYS:HD3	1.52	0.90
1:E:445:ARG:HB3	1:E:464:LEU:HB3	1.52	0.90
1:G:105:PRO:HB2	1:G:107:GLN:HG2	1.52	0.89
1:H:29:ILE:HG22	1:H:31:GLY:H	1.36	0.89
1:G:309:ARG:HD3	1:G:309:ARG:H	1.38	0.89
1:H:115:LYS:HA	1:H:118:GLN:HG3	1.53	0.89
1:B:38:ASP:OD1	2:B:601:FAD:H1B	1.73	0.88
1:E:162:TYR:O	1:E:166:VAL:HG12	1.73	0.88
1:H:376:GLU:HG3	1:H:382:VAL:HG13	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:188:LEU:O	1:F:192:THR:HG23	1.74	0.88
1:G:17:PRO:CD	2:G:601:FAD:O1P	2.20	0.88
1:G:121:CYS:HB3	1:G:154:ILE:HG13	1.56	0.88
1:C:332:SER:HA	1:C:339:GLN:NE2	1.89	0.88
1:G:445:ARG:HA	1:G:450:SER:HB2	1.53	0.88
1:H:455:VAL:O	1:H:460:HIS:HB3	1.74	0.88
1:H:47:ALA:HB3	1:H:222:TRP:HE1	1.36	0.87
1:E:149:MET:SD	1:E:186:PRO:HD2	2.14	0.87
1:C:110:ILE:HA	1:C:113:LEU:HD12	1.57	0.87
1:H:271:VAL:HG12	1:H:448:PHE:O	1.75	0.87
1:H:59:ASP:HB3	1:H:63:HIS:HD2	1.40	0.87
1:H:309:ARG:H	1:H:309:ARG:HD3	1.41	0.86
1:D:122:ILE:O	1:D:126:ILE:HG13	1.76	0.86
1:B:110:ILE:HA	1:B:113:LEU:HD12	1.57	0.86
1:G:121:CYS:HA	1:G:153:GLY:HA3	1.58	0.86
1:G:69:TYR:CD2	1:G:463:MET:HG3	2.11	0.86
1:D:178:TRP:HB2	1:D:454:GLU:HG3	1.57	0.86
1:D:105:PRO:O	1:D:109:ASN:ND2	2.09	0.86
1:C:178:TRP:HB2	1:C:454:GLU:HG3	1.57	0.86
1:G:376:GLU:HG3	1:G:382:VAL:HG13	1.57	0.86
1:G:150:MET:HG3	1:G:154:ILE:HB	1.58	0.85
1:B:193:THR:HG23	1:H:119:VAL:HG11	1.58	0.85
1:C:494:GLU:HG2	1:G:477:VAL:HA	1.56	0.85
1:E:9:ASP:HA	1:E:263:LYS:HD3	1.57	0.85
1:A:122:ILE:O	1:A:126:ILE:HG13	1.77	0.85
1:B:178:TRP:HB2	1:B:454:GLU:HG3	1.57	0.85
1:E:63:HIS:CE1	2:E:601:FAD:C9A	2.59	0.85
1:A:111:SER:HB3	1:A:198:GLY:HA2	1.58	0.85
1:A:243:THR:HB	1:F:243:THR:HG21	1.56	0.85
3:A:602:GDU:H6	3:A:602:GDU:H5'1	1.59	0.84
1:F:56:PHE:CE1	1:F:339:GLN:HB3	2.12	0.84
1:G:91:ARG:HH21	1:G:203:ASN:HA	1.40	0.84
2:A:601:FAD:H9	2:A:601:FAD:O2'	1.77	0.84
1:G:149:MET:SD	1:G:184:ALA:HA	2.17	0.84
1:H:121:CYS:HA	1:H:153:GLY:HA3	1.60	0.84
1:D:332:SER:HA	1:D:339:GLN:NE2	1.92	0.84
1:H:332:SER:HA	1:H:339:GLN:NE2	1.92	0.84
1:G:17:PRO:HD2	2:G:601:FAD:O1A	1.78	0.83
1:E:154:ILE:H	1:E:154:ILE:HD13	1.44	0.83
1:G:281:GLN:OE1	1:G:281:GLN:HA	1.75	0.83
1:F:175:GLN:OE1	1:F:178:TRP:HD1	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:VAL:HG23	1:E:196:ILE:HG21	1.61	0.83
1:H:109:ASN:ND2	1:H:201:ALA:O	2.12	0.83
1:E:455:VAL:HA	1:E:460:HIS:HD1	1.44	0.82
1:H:121:CYS:HB3	1:H:154:ILE:HG13	1.61	0.82
1:H:57:LEU:HD11	1:H:338:ASN:HA	1.61	0.82
1:F:187:ASN:OD1	1:F:189:LYS:HB2	1.79	0.82
1:A:178:TRP:HB2	1:A:454:GLU:HG3	1.60	0.82
1:A:280:ASP:O	1:A:284:VAL:HG23	1.78	0.82
1:E:458:GLN:HG3	2:E:601:FAD:H2'	1.62	0.82
1:E:332:SER:HA	1:E:339:GLN:NE2	1.95	0.82
1:E:338:ASN:HB2	1:E:339:GLN:NE2	1.94	0.81
1:H:69:TYR:CD2	1:H:463:MET:HG3	2.16	0.81
1:G:411:TYR:HD1	1:G:412:HIS:N	1.78	0.81
1:B:332:SER:HA	1:B:339:GLN:NE2	1.94	0.81
1:A:332:SER:HA	1:A:339:GLN:NE2	1.94	0.81
1:D:91:ARG:HG3	1:D:315:TRP:CH2	2.16	0.81
1:H:468:ALA:O	1:H:471:ASN:HB3	1.80	0.81
1:A:244:LYS:HB2	1:F:255:GLN:NE2	1.96	0.81
1:F:430:LEU:HD22	1:F:434:LEU:HG	1.61	0.81
1:E:281:GLN:HA	1:E:281:GLN:OE1	1.79	0.81
1:G:332:SER:HA	1:G:339:GLN:NE2	1.96	0.80
1:D:16:GLY:HA3	2:D:601:FAD:H52A	1.62	0.80
1:B:111:SER:HB3	1:B:198:GLY:HA2	1.64	0.80
1:D:91:ARG:HD3	1:D:207:ASN:HB2	1.64	0.80
1:A:350:GLN:HE22	1:A:354:GLY:HA2	1.46	0.80
1:F:70:LYS:HG3	1:F:496:ARG:NH2	1.93	0.80
1:G:197:LEU:C	1:G:199:LYS:N	2.35	0.80
1:F:467:GLU:HG3	1:F:495:ARG:NH1	1.96	0.80
1:D:280:ASP:O	1:D:284:VAL:HG23	1.81	0.80
1:F:27:ASN:HB2	1:F:34:TRP:CZ2	2.16	0.80
1:H:411:TYR:HD1	1:H:412:HIS:N	1.80	0.80
1:E:457:ASN:HB3	2:E:601:FAD:C2	2.12	0.79
1:D:458:GLN:HG3	2:D:601:FAD:H2'	1.63	0.79
1:H:144:GLU:O	1:H:148:ARG:HG3	1.83	0.79
1:H:105:PRO:HB2	1:H:107:GLN:HG2	1.64	0.79
1:F:63:HIS:H	1:F:63:HIS:CD2	1.98	0.79
1:H:271:VAL:N	1:H:448:PHE:O	2.14	0.79
1:G:57:LEU:HD11	1:G:338:ASN:HA	1.65	0.79
1:H:389:ALA:HA	1:H:392:ILE:HD12	1.63	0.79
1:G:154:ILE:HD12	1:G:154:ILE:H	1.45	0.79
1:H:417:HIS:HB3	1:H:448:PHE:CE2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:51:VAL:HG22	1:G:57:LEU:HB3	1.64	0.78
1:C:91:ARG:HG3	1:C:315:TRP:CH2	2.19	0.78
1:A:110:ILE:HA	1:A:113:LEU:HD12	1.64	0.78
1:G:218:THR:HA	1:G:221:ILE:HD12	1.64	0.78
1:A:188:LEU:O	1:A:192:THR:HG23	1.83	0.78
1:G:346:LEU:HD23	1:G:347:PRO:HD2	1.65	0.78
1:D:111:SER:HB3	1:D:198:GLY:HA2	1.65	0.78
1:G:29:ILE:HG22	1:G:31:GLY:H	1.49	0.78
1:A:91:ARG:HH12	1:A:205:GLY:HA3	1.49	0.78
1:H:418:GLY:C	1:H:419:TYR:HD1	1.86	0.78
1:F:230:PRO:HG2	1:F:233:LYS:HD2	1.66	0.78
1:E:188:LEU:O	1:E:192:THR:HG23	1.84	0.78
1:B:398:THR:HG22	1:B:400:MET:HG2	1.64	0.78
1:H:359:SER:HB3	1:H:363:LYS:HE2	1.66	0.78
1:G:314:CYS:HB3	1:G:315:TRP:HE3	1.49	0.78
1:E:22:ALA:HA	1:E:469:VAL:CG2	2.14	0.77
1:H:194:ASN:ND2	1:H:199:LYS:HB3	1.99	0.77
1:F:178:TRP:HB2	1:F:454:GLU:HG3	1.65	0.77
1:D:110:ILE:HA	1:D:113:LEU:HD12	1.67	0.77
1:G:18:THR:HG22	1:G:268:THR:CG2	2.14	0.77
1:A:91:ARG:HD3	1:A:207:ASN:HB2	1.67	0.77
1:B:122:ILE:O	1:B:126:ILE:HG13	1.84	0.77
1:H:314:CYS:HB3	1:H:315:TRP:HE3	1.49	0.77
1:H:17:PRO:HG3	1:H:222:TRP:CZ2	2.20	0.77
1:C:188:LEU:O	1:C:192:THR:HG23	1.84	0.77
1:F:151:GLY:O	1:F:154:ILE:HG12	1.85	0.77
1:G:79:ALA:HB2	1:G:225:VAL:HG23	1.65	0.77
1:B:188:LEU:O	1:B:192:THR:HG23	1.85	0.77
1:A:420:PRO:HG2	1:A:453:TYR:HB2	1.66	0.77
1:C:398:THR:O	1:C:398:THR:HG22	1.84	0.77
1:G:18:THR:CG2	1:G:268:THR:HG21	2.14	0.77
1:H:51:VAL:HG22	1:H:57:LEU:HB3	1.66	0.77
1:C:122:ILE:O	1:C:126:ILE:HG13	1.84	0.76
1:H:249:ASN:HB2	1:H:251:THR:HG23	1.66	0.76
1:F:101:TRP:CZ3	1:F:316:LEU:HD13	2.19	0.76
1:G:96:ARG:HG2	1:G:398:THR:HG22	1.67	0.76
1:H:47:ALA:HB3	1:H:222:TRP:NE1	2.00	0.76
1:F:108:ASN:HB3	1:F:194:ASN:ND2	2.00	0.76
1:E:398:THR:OG1	1:E:400:MET:HG2	1.85	0.76
1:F:332:SER:HA	1:F:339:GLN:NE2	1.99	0.76
1:A:91:ARG:HG3	1:A:315:TRP:CH2	2.20	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:SER:HB3	1:C:198:GLY:HA2	1.67	0.76
1:E:353:ASP:HB3	1:E:403:PRO:CB	2.15	0.76
1:E:267:SER:O	1:E:444:SER:HA	1.86	0.76
1:F:149:MET:SD	1:F:186:PRO:HD2	2.25	0.76
1:G:468:ALA:O	1:G:471:ASN:HB3	1.84	0.76
1:E:19:GLY:N	1:E:268:THR:HG21	2.01	0.76
1:E:280:ASP:O	1:E:284:VAL:HG23	1.86	0.76
1:G:348:THR:O	1:G:357:PRO:HG3	1.85	0.76
1:F:22:ALA:HA	1:F:469:VAL:CG2	2.15	0.76
1:E:178:TRP:HB2	1:E:454:GLU:HG3	1.65	0.76
1:F:338:ASN:HB2	1:F:339:GLN:NE2	2.01	0.75
1:H:130:LEU:O	1:H:133:ARG:HB3	1.86	0.75
1:G:18:THR:CG2	1:G:268:THR:CG2	2.63	0.75
1:E:127:ASP:O	1:E:131:GLU:HG2	1.86	0.75
1:H:155:ALA:O	1:H:160:ARG:HG3	1.86	0.75
1:G:47:ALA:HB3	1:G:222:TRP:NE1	2.02	0.75
1:E:56:PHE:CE1	1:E:339:GLN:HB3	2.21	0.75
1:A:414:ARG:HD3	1:F:281:GLN:HB3	1.68	0.75
1:G:351:LEU:O	1:G:354:GLY:N	2.19	0.75
1:B:91:ARG:HD3	1:B:207:ASN:HB2	1.67	0.75
1:F:91:ARG:HD3	1:F:207:ASN:HB2	1.67	0.75
1:A:60:VAL:O	1:A:63:HIS:NE2	2.20	0.75
1:C:280:ASP:O	1:C:284:VAL:HG23	1.86	0.75
1:B:47:ALA:HB1	1:B:222:TRP:HE1	1.51	0.75
1:H:446:GLY:H	1:H:450:SER:HB3	1.52	0.75
1:D:188:LEU:O	1:D:192:THR:HG23	1.87	0.74
1:F:80:LEU:HD12	1:F:86:TRP:CZ2	2.22	0.74
1:D:420:PRO:HG2	1:D:453:TYR:HB2	1.69	0.74
1:G:271:VAL:HG12	1:G:448:PHE:O	1.87	0.74
1:G:338:ASN:HB2	1:G:339:GLN:NE2	2.03	0.74
1:F:127:ASP:O	1:F:131:GLU:HG2	1.88	0.74
1:H:393:GLN:O	1:H:396:VAL:N	2.19	0.74
1:B:280:ASP:O	1:B:284:VAL:HG23	1.86	0.74
1:G:109:ASN:ND2	1:G:201:ALA:O	2.21	0.74
1:E:60:VAL:O	1:E:63:HIS:NE2	2.21	0.74
1:D:462:PHE:O	1:D:466:VAL:HG23	1.88	0.74
1:G:393:GLN:O	1:G:396:VAL:N	2.19	0.74
1:D:104:TYR:CD1	1:D:105:PRO:HA	2.22	0.73
1:G:249:ASN:HB2	1:G:251:THR:HG23	1.69	0.73
1:G:17:PRO:HG3	1:G:222:TRP:CZ2	2.22	0.73
1:G:271:VAL:N	1:G:448:PHE:O	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:443:TRP:HA	1:H:445:ARG:HH21	1.54	0.73
1:E:71:TYR:O	1:E:74:ASP:HB2	1.87	0.73
1:E:383:ASN:HB3	1:E:386:THR:OG1	1.88	0.73
1:H:338:ASN:HB2	1:H:339:GLN:NE2	2.03	0.73
1:H:303:ARG:NH1	1:H:406:GLU:OE2	2.21	0.73
1:B:159:MET:HE3	3:B:602:GDU:HN3	1.53	0.73
1:B:91:ARG:HG3	1:B:315:TRP:CH2	2.24	0.73
1:B:108:ASN:N	1:B:108:ASN:OD1	2.20	0.73
1:H:79:ALA:HB2	1:H:225:VAL:HG23	1.70	0.73
1:G:418:GLY:C	1:G:419:TYR:HD1	1.91	0.72
1:C:421:THR:HG22	1:C:423:THR:HG23	1.69	0.72
1:G:104:TYR:O	1:G:203:ASN:N	2.22	0.72
1:F:93:SER:OG	1:F:315:TRP:NE1	2.22	0.72
1:G:37:VAL:HG12	1:G:235:ARG:HB2	1.71	0.72
1:F:303:ARG:HH21	1:F:363:LYS:HB2	1.52	0.72
1:G:18:THR:HG21	1:G:268:THR:HG22	1.72	0.72
1:E:471:ASN:ND2	1:E:476:ALA:O	2.20	0.72
1:B:130:LEU:HD23	1:H:130:LEU:HD23	1.72	0.72
1:G:181:GLU:N	1:G:485:ASP:OD1	2.21	0.72
1:B:420:PRO:HG2	1:B:453:TYR:HB2	1.70	0.72
1:E:91:ARG:HD3	1:E:207:ASN:HB2	1.71	0.72
1:G:48:SER:O	1:G:60:VAL:HG23	1.89	0.72
1:C:104:TYR:CD1	1:C:105:PRO:HA	2.25	0.72
1:A:104:TYR:CD1	1:A:105:PRO:HA	2.23	0.72
1:E:80:LEU:HD12	1:E:86:TRP:CZ2	2.23	0.72
1:C:350:GLN:HE22	1:C:354:GLY:HA2	1.55	0.72
1:H:402:LYS:NZ	1:H:405:ASP:OD1	2.21	0.72
1:F:398:THR:OG1	1:F:400:MET:HG2	1.90	0.72
1:E:465:GLY:O	1:E:469:VAL:HG23	1.90	0.72
1:E:457:ASN:HA	2:E:601:FAD:H1'2	1.71	0.72
1:C:303:ARG:NH2	1:C:363:LYS:O	2.22	0.72
1:E:303:ARG:NH2	1:E:363:LYS:HG3	2.04	0.72
1:E:133:ARG:NH1	1:E:133:ARG:HG3	2.03	0.72
1:F:19:GLY:N	1:F:268:THR:HG21	2.04	0.71
1:G:417:HIS:HB3	1:G:448:PHE:CE2	2.24	0.71
1:H:59:ASP:HB3	1:H:63:HIS:CD2	2.23	0.71
1:G:142:PHE:HB3	1:G:171:THR:O	1.89	0.71
1:A:104:TYR:HE1	3:A:602:GDU:C5	2.03	0.71
1:D:91:ARG:HH12	1:D:205:GLY:HA3	1.54	0.71
1:E:230:PRO:HG2	1:E:233:LYS:HD2	1.71	0.71
1:E:9:ASP:O	1:E:263:LYS:HB2	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:LEU:O	1:G:133:ARG:HB3	1.90	0.71
1:F:494:GLU:CD	1:F:494:GLU:H	1.91	0.71
1:C:420:PRO:HG2	1:C:453:TYR:HB2	1.70	0.71
1:F:353:ASP:HB3	1:F:403:PRO:CB	2.20	0.71
1:F:465:GLY:O	1:F:469:VAL:HG23	1.90	0.71
1:G:314:CYS:HB3	1:G:315:TRP:CE3	2.26	0.71
1:H:181:GLU:OE1	1:H:181:GLU:HA	1.91	0.71
1:A:462:PHE:O	1:A:466:VAL:HG23	1.89	0.71
1:H:212:PHE:CG	1:H:213:PRO:HD2	2.25	0.71
1:G:143:ASP:HA	1:G:146:ILE:HD12	1.71	0.71
1:C:91:ARG:HD3	1:C:207:ASN:HB2	1.73	0.71
1:A:421:THR:HG22	1:A:423:THR:HG23	1.72	0.71
1:H:188:LEU:O	1:H:192:THR:HG23	1.90	0.71
1:G:188:LEU:O	1:G:192:THR:HG23	1.91	0.71
1:A:473:VAL:O	1:E:499:ASP:HB3	1.91	0.71
1:E:122:ILE:O	1:E:126:ILE:HG13	1.91	0.71
1:G:447:ARG:O	1:G:451:TRP:HA	1.91	0.71
1:F:27:ASN:HB2	1:F:34:TRP:HZ2	1.55	0.70
1:B:183:VAL:HG22	3:B:602:GDU:C1D	2.18	0.70
1:H:218:THR:HA	1:H:221:ILE:HD12	1.73	0.70
1:G:28:GLN:HE21	1:G:497:LEU:C	1.93	0.70
1:G:303:ARG:NH1	1:G:406:GLU:OE2	2.23	0.70
1:E:265:LEU:HD23	1:E:442:ILE:HG12	1.72	0.70
1:H:482:ASN:HB2	1:H:483:TYR:CE2	2.27	0.70
1:G:171:THR:HA	1:G:174:MET:HE2	1.72	0.70
1:H:54:GLU:HB3	1:H:346:LEU:HD11	1.71	0.70
1:A:455:VAL:O	1:A:460:HIS:HB3	1.90	0.70
1:G:392:ILE:O	1:G:395:LEU:HB2	1.92	0.70
1:E:70:LYS:HB3	1:E:496:ARG:HH12	1.56	0.70
1:H:467:GLU:OE1	1:H:480:THR:N	2.21	0.70
1:C:115:LYS:HD3	1:E:196:ILE:O	1.90	0.70
1:H:37:VAL:HG12	1:H:235:ARG:HB2	1.73	0.70
1:D:463:MET:O	1:D:467:GLU:HG3	1.92	0.70
1:B:419:TYR:HE1	2:B:601:FAD:HM73	1.54	0.70
1:E:142:PHE:O	1:E:145:TRP:HB3	1.91	0.70
1:G:468:ALA:O	1:G:472:ILE:HD12	1.92	0.70
1:F:303:ARG:HH21	1:F:363:LYS:CB	2.05	0.70
1:G:25:ARG:HH11	1:G:470:ASP:CG	1.94	0.70
1:F:267:SER:O	1:F:444:SER:HA	1.90	0.70
1:H:96:ARG:HG2	1:H:398:THR:HG22	1.74	0.70
1:C:47:ALA:HB1	1:C:222:TRP:HE1	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:440:LYS:HB2	1:H:442:ILE:HD12	1.74	0.70
1:H:274:LEU:O	1:H:278:MET:HG2	1.92	0.70
1:C:103:PRO:HG2	1:C:109:ASN:ND2	2.06	0.70
1:G:445:ARG:HA	1:G:450:SER:CB	2.21	0.70
1:G:142:PHE:O	1:G:146:ILE:HG13	1.92	0.70
1:A:91:ARG:NH2	1:A:204:TRP:O	2.24	0.70
1:E:175:GLN:HE22	1:E:177:ALA:HB3	1.56	0.69
1:H:84:ASP:OD2	1:H:84:ASP:N	2.22	0.69
1:E:455:VAL:HG23	1:E:455:VAL:O	1.91	0.69
1:H:308:GLU:HG3	1:H:309:ARG:HD3	1.74	0.69
1:H:107:GLN:CD	1:H:107:GLN:H	1.94	0.69
1:B:350:GLN:HE22	1:B:354:GLY:HA2	1.57	0.69
1:B:104:TYR:CD1	1:B:105:PRO:HA	2.28	0.69
1:E:118:GLN:OE1	1:E:195:VAL:HG13	1.92	0.69
1:B:176:CYS:O	1:B:179:LEU:HD12	1.93	0.69
1:H:484:PRO:HA	1:H:487:VAL:HG22	1.74	0.69
1:F:280:ASP:O	1:F:284:VAL:HG23	1.93	0.69
1:H:103:PRO:HB2	1:H:202:GLY:HA2	1.75	0.69
1:G:84:ASP:OD2	1:G:84:ASP:N	2.24	0.69
1:E:22:ALA:HA	1:E:469:VAL:HG22	1.75	0.69
1:G:207:ASN:OD1	1:G:207:ASN:C	2.31	0.69
1:G:144:GLU:O	1:G:148:ARG:HG3	1.93	0.69
1:B:398:THR:O	1:B:398:THR:CG2	2.40	0.69
1:H:314:CYS:HB3	1:H:315:TRP:CE3	2.26	0.69
1:B:91:ARG:HH12	1:B:205:GLY:HA3	1.56	0.69
1:E:313:LYS:O	1:E:333:ASN:ND2	2.26	0.69
1:G:159:MET:O	1:G:163:ASN:HB2	1.91	0.69
1:D:421:THR:HG22	1:D:423:THR:HG23	1.74	0.69
1:E:419:TYR:HE1	2:E:601:FAD:HM73	1.58	0.69
1:F:105:PRO:O	1:F:109:ASN:ND2	2.26	0.69
1:F:163:ASN:OD1	3:F:602:GDU:O3D	2.09	0.69
1:F:63:HIS:HD2	1:F:63:HIS:H	1.40	0.69
1:G:389:ALA:HA	1:G:392:ILE:HD12	1.75	0.69
1:C:455:VAL:O	1:C:460:HIS:HB3	1.93	0.69
1:E:350:GLN:O	1:E:407:ILE:HB	1.93	0.68
1:F:133:ARG:NH1	1:F:133:ARG:HG3	2.04	0.68
1:G:322:ASN:HD22	1:G:397:ASN:HB3	1.58	0.68
1:G:492:ASN:HD22	1:G:492:ASN:H	1.42	0.68
1:G:341:GLU:HG3	1:G:343:SER:H	1.59	0.68
1:H:203:ASN:HD22	1:H:204:TRP:H	1.39	0.68
1:E:18:THR:OG1	1:E:461:SER:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:54:GLU:HB3	1:G:346:LEU:HD11	1.76	0.68
1:H:142:PHE:O	1:H:146:ILE:HG13	1.93	0.68
1:H:445:ARG:HA	1:H:450:SER:HB2	1.73	0.68
1:E:101:TRP:CZ3	1:E:316:LEU:HD13	2.29	0.68
1:C:429:ALA:O	1:C:433:ILE:HD12	1.93	0.68
1:C:19:GLY:N	1:C:268:THR:HG21	2.09	0.68
1:E:104:TYR:HE1	3:E:602:GDU:C5	2.06	0.68
1:G:331:PHE:CD2	1:G:338:ASN:HB3	2.29	0.68
1:C:462:PHE:O	1:C:466:VAL:HG23	1.93	0.68
1:E:143:ASP:HA	1:E:146:ILE:HD12	1.76	0.68
1:C:136:ASN:OD1	1:C:137:THR:HG23	1.92	0.68
1:H:159:MET:O	1:H:163:ASN:HB2	1.93	0.68
1:C:453:TYR:OH	3:C:602:GDU:O3A	2.10	0.68
1:G:245:VAL:O	1:G:278:MET:HA	1.93	0.68
1:E:27:ASN:HB2	1:E:34:TRP:CZ2	2.29	0.68
1:B:40:ASN:O	1:B:236:PHE:HB3	1.94	0.68
1:H:68:HIS:O	1:H:492:ASN:ND2	2.27	0.68
1:H:60:VAL:O	1:H:63:HIS:NE2	2.27	0.68
1:E:93:SER:OG	1:E:315:TRP:NE1	2.27	0.68
1:D:455:VAL:O	1:D:460:HIS:HB3	1.93	0.68
1:A:18:THR:OG1	1:A:461:SER:HB3	1.94	0.68
1:D:54:GLU:HB3	1:D:346:LEU:HD11	1.76	0.67
1:B:462:PHE:O	1:B:466:VAL:HG23	1.94	0.67
1:F:71:TYR:O	1:F:74:ASP:HB2	1.93	0.67
1:H:281:GLN:HA	1:H:281:GLN:OE1	1.93	0.67
1:F:431:THR:O	1:F:435:PRO:HG2	1.94	0.67
1:E:16:GLY:HA3	2:E:601:FAD:O1P	1.94	0.67
1:F:5:ASP:H	1:F:259:THR:HG1	1.40	0.67
1:E:12:VAL:HB	1:E:36:ILE:HG13	1.75	0.67
1:E:437:LEU:HB3	1:E:442:ILE:HB	1.75	0.67
1:C:103:PRO:HB2	1:C:109:ASN:ND2	2.10	0.67
1:B:421:THR:HG22	1:B:423:THR:HG23	1.76	0.67
1:B:271:VAL:HA	1:B:274:LEU:HB2	1.77	0.67
1:B:142:PHE:O	1:B:146:ILE:HG13	1.94	0.67
1:G:445:ARG:NH1	1:G:481:LEU:HD22	2.10	0.67
1:H:447:ARG:O	1:H:451:TRP:HA	1.95	0.67
1:B:107:GLN:NE2	3:B:602:GDU:O4	2.27	0.67
1:G:204:TRP:HB3	1:G:208:ALA:HB2	1.76	0.67
1:F:122:ILE:HG23	1:F:126:ILE:HD11	1.76	0.67
1:D:91:ARG:NH1	1:D:205:GLY:HA3	2.09	0.67
1:D:63:HIS:CD2	2:D:601:FAD:C5X	2.78	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LYS:HB3	1:F:197:LEU:HD23	1.77	0.67
1:G:353:ASP:HB3	1:G:403:PRO:HB3	1.77	0.67
1:F:336:PRO:HG2	1:F:337:TYR:CD1	2.30	0.67
1:A:136:ASN:OD1	1:A:137:THR:HG23	1.95	0.67
1:B:159:MET:CE	3:B:602:GDU:HN3	2.08	0.67
1:B:398:THR:HG22	1:B:398:THR:O	1.93	0.67
1:H:297:VAL:HB	1:H:415:PHE:HE2	1.59	0.67
1:E:179:LEU:HD23	1:E:179:LEU:N	2.09	0.67
1:E:494:GLU:CD	1:E:494:GLU:H	1.98	0.67
1:B:43:PRO:HG2	1:B:223:ILE:HD13	1.77	0.67
1:A:358:GLN:OE1	1:A:358:GLN:N	2.28	0.67
1:B:91:ARG:NH2	1:B:204:TRP:O	2.28	0.67
1:C:108:ASN:OD1	1:C:108:ASN:N	2.21	0.67
1:H:392:ILE:O	1:H:395:LEU:HB2	1.95	0.67
1:G:155:ALA:O	1:G:160:ARG:HG3	1.95	0.67
1:A:58:TYR:HA	1:A:331:PHE:HE2	1.59	0.67
1:E:187:ASN:OD1	1:E:189:LYS:HB2	1.95	0.67
1:F:184:ALA:HA	1:F:204:TRP:CZ2	2.29	0.67
1:F:104:TYR:CE1	3:F:602:GDU:O4	2.48	0.66
1:E:17:PRO:O	1:E:462:PHE:HA	1.95	0.66
1:F:142:PHE:O	1:F:145:TRP:HB3	1.95	0.66
1:F:91:ARG:HG3	1:F:315:TRP:CH2	2.29	0.66
1:C:303:ARG:HH21	1:C:363:LYS:C	1.98	0.66
1:F:12:VAL:HB	1:F:36:ILE:HG13	1.76	0.66
1:H:57:LEU:CD1	1:H:338:ASN:HA	2.25	0.66
1:B:119:VAL:HG22	1:H:193:THR:HG22	1.76	0.66
1:A:54:GLU:HB3	1:A:346:LEU:HD11	1.77	0.66
1:A:45:GLY:HA3	2:A:601:FAD:O1A	1.96	0.66
1:E:429:ALA:O	1:E:433:ILE:HG13	1.95	0.66
1:D:63:HIS:HD2	2:D:601:FAD:C5X	2.08	0.66
1:F:281:GLN:OE1	1:F:281:GLN:HA	1.96	0.66
1:H:204:TRP:HA	1:H:204:TRP:CE3	2.29	0.66
1:E:457:ASN:HB3	2:E:601:FAD:O2	1.94	0.66
1:G:306:ARG:HH11	1:G:312:ASP:HA	1.61	0.66
1:D:46:LEU:HG	2:D:601:FAD:O1A	1.95	0.66
1:E:353:ASP:HB3	1:E:403:PRO:HB2	1.77	0.66
1:C:176:CYS:O	1:C:179:LEU:HD12	1.96	0.66
1:E:269:MET:HE2	1:E:273:PHE:HB3	1.76	0.66
1:G:149:MET:O	1:G:186:PRO:HB3	1.95	0.66
1:G:432:GLN:O	1:G:436:LYS:HG2	1.96	0.66
1:G:308:GLU:HG3	1:G:309:ARG:HD3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:47:ALA:HB2	2:H:601:FAD:H4'	1.78	0.66
1:E:430:LEU:HD22	1:E:434:LEU:HG	1.77	0.66
1:D:271:VAL:HG12	1:D:448:PHE:O	1.95	0.66
1:G:446:GLY:H	1:G:450:SER:HB3	1.60	0.66
1:H:306:ARG:HD2	1:H:311:GLY:O	1.94	0.66
1:G:254:LEU:HG	1:G:258:THR:HG22	1.78	0.66
1:H:9:ASP:HA	1:H:263:LYS:HD3	1.78	0.66
1:G:58:TYR:CE2	1:G:299:GLY:HA3	2.31	0.66
1:D:458:GLN:HA	2:D:601:FAD:O3'	1.97	0.66
1:G:345:LYS:HD3	1:G:364:GLU:HG2	1.77	0.66
1:C:58:TYR:HA	1:C:331:PHE:HE2	1.59	0.66
1:E:326:TYR:CD2	1:E:374:VAL:HA	2.31	0.65
1:E:349:MET:N	1:E:407:ILE:O	2.27	0.65
1:F:383:ASN:HB3	1:F:386:THR:OG1	1.96	0.65
1:B:455:VAL:O	1:B:460:HIS:HB3	1.95	0.65
1:B:108:ASN:ND2	1:B:201:ALA:HB3	2.11	0.65
1:B:19:GLY:N	1:B:268:THR:HG21	2.11	0.65
1:E:137:THR:O	1:E:148:ARG:NH1	2.28	0.65
1:E:336:PRO:HG2	1:E:337:TYR:CD1	2.31	0.65
1:A:91:ARG:NH1	1:A:205:GLY:HA3	2.11	0.65
1:H:139:PRO:HB2	1:H:176:CYS:SG	2.36	0.65
1:H:325:PHE:CD2	1:H:372:LEU:HD22	2.31	0.65
1:G:162:TYR:CZ	1:G:166:VAL:HG11	2.31	0.65
1:F:413:ARG:HD3	1:F:415:PHE:CE2	2.31	0.65
1:H:346:LEU:HD23	1:H:347:PRO:HD2	1.78	0.65
1:H:71:TYR:CD2	1:H:495:ARG:HG2	2.32	0.65
1:F:331:PHE:CE2	1:F:338:ASN:ND2	2.65	0.65
1:E:51:VAL:HA	1:E:56:PHE:O	1.97	0.65
1:H:245:VAL:O	1:H:278:MET:HA	1.97	0.65
1:F:429:ALA:O	1:F:433:ILE:HG13	1.97	0.65
1:A:336:PRO:HG2	1:A:337:TYR:CE1	2.31	0.65
1:B:69:TYR:CG	1:B:463:MET:HG3	2.32	0.65
1:H:29:ILE:HG22	1:H:31:GLY:N	2.12	0.64
1:F:440:LYS:HB2	1:F:442:ILE:HD12	1.79	0.64
1:F:419:TYR:HE1	2:F:601:FAD:HM73	1.62	0.64
1:C:40:ASN:O	1:C:236:PHE:HB3	1.97	0.64
1:F:51:VAL:HA	1:F:56:PHE:O	1.96	0.64
1:H:348:THR:O	1:H:357:PRO:HG3	1.96	0.64
1:E:368:TRP:CZ3	1:E:370:ILE:HD11	2.32	0.64
1:D:47:ALA:HB1	1:D:222:TRP:HE1	1.63	0.64
1:D:136:ASN:OD1	1:D:137:THR:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:TYR:CD2	1:F:374:VAL:HA	2.32	0.64
1:D:108:ASN:N	1:D:108:ASN:OD1	2.20	0.64
1:C:144:GLU:O	1:C:148:ARG:HG3	1.98	0.64
1:D:398:THR:HB	1:D:400:MET:CG	2.28	0.64
1:H:21:GLY:HA2	1:H:462:PHE:CE1	2.32	0.64
1:G:44:GLY:HA3	1:G:222:TRP:CD1	2.33	0.64
1:C:119:VAL:HA	1:E:196:ILE:HD13	1.78	0.64
1:F:179:LEU:N	1:F:179:LEU:HD23	2.12	0.64
1:D:69:TYR:CG	1:D:463:MET:HG3	2.33	0.64
1:C:43:PRO:HG2	1:C:223:ILE:HD13	1.80	0.64
1:F:18:THR:OG1	1:F:461:SER:HB3	1.97	0.64
1:H:484:PRO:O	1:H:488:ASN:HB2	1.96	0.64
1:C:91:ARG:HH12	1:C:205:GLY:HA3	1.61	0.64
1:H:251:THR:HA	1:H:260:ILE:O	1.98	0.64
1:E:175:GLN:NE2	1:E:177:ALA:H	1.94	0.64
1:E:184:ALA:HA	1:E:204:TRP:CZ2	2.32	0.64
1:F:17:PRO:HD2	2:F:601:FAD:O5'	1.98	0.64
1:A:197:LEU:HD23	1:G:115:LYS:HD3	1.80	0.64
1:G:91:ARG:HH21	1:G:203:ASN:CA	2.11	0.64
1:C:69:TYR:CG	1:C:463:MET:HG3	2.33	0.64
1:E:115:LYS:O	1:E:119:VAL:HG23	1.97	0.64
1:G:71:TYR:CD2	1:G:495:ARG:HG2	2.33	0.64
1:C:271:VAL:HG12	1:C:448:PHE:O	1.98	0.64
1:G:484:PRO:O	1:G:488:ASN:HB2	1.97	0.63
1:F:184:ALA:HB2	1:F:204:TRP:CD2	2.32	0.63
1:B:11:LEU:O	1:B:265:LEU:HD12	1.99	0.63
1:A:325:PHE:HA	1:A:374:VAL:HG22	1.80	0.63
1:F:457:ASN:HB3	2:F:601:FAD:C2	2.28	0.63
1:H:268:THR:HA	1:H:445:ARG:O	1.98	0.63
1:F:56:PHE:HE1	1:F:339:GLN:HB3	1.62	0.63
1:G:58:TYR:HD2	1:G:411:TYR:HD2	1.46	0.63
1:H:171:THR:HA	1:H:174:MET:HE2	1.79	0.63
1:B:104:TYR:HE1	3:B:602:GDU:H5	1.62	0.63
1:G:44:GLY:CA	1:G:222:TRP:CD1	2.81	0.63
1:H:336:PRO:HG2	1:H:337:TYR:CE1	2.33	0.63
1:B:504:PHE:HZ	1:F:264:LYS:HG2	1.63	0.63
1:D:301:GLY:HA3	1:D:409:SER:HB3	1.80	0.63
1:E:413:ARG:HD3	1:E:415:PHE:CE2	2.32	0.63
1:E:326:TYR:H	1:E:374:VAL:HG13	1.64	0.63
1:H:142:PHE:HB3	1:H:171:THR:O	1.98	0.63
1:G:103:PRO:HB2	1:G:109:ASN:ND2	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:TYR:HA	1:B:331:PHE:HE2	1.63	0.63
1:E:16:GLY:HA3	2:E:601:FAD:O5B	1.98	0.63
1:A:69:TYR:CG	1:A:463:MET:HG3	2.34	0.63
1:G:326:TYR:CE2	1:G:375:SER:HB3	2.32	0.63
1:B:486:PHE:HE1	1:F:483:TYR:CD1	2.16	0.63
1:F:97:CYS:SG	1:F:98:GLN:HG3	2.38	0.63
1:H:326:TYR:HE2	1:H:375:SER:N	1.96	0.63
1:D:19:GLY:N	1:D:268:THR:HG21	2.13	0.63
1:F:142:PHE:O	1:F:146:ILE:HG13	1.99	0.63
1:F:63:HIS:N	1:F:63:HIS:CD2	2.66	0.63
1:A:176:CYS:O	1:A:179:LEU:HD12	1.98	0.63
1:C:103:PRO:O	1:C:109:ASN:ND2	2.26	0.63
1:E:348:THR:OG1	1:E:406:GLU:HB3	1.99	0.63
1:C:17:PRO:HD2	2:C:601:FAD:O5'	1.98	0.63
1:H:322:ASN:HD22	1:H:397:ASN:HB3	1.64	0.63
1:F:143:ASP:HA	1:F:146:ILE:HD12	1.80	0.62
1:G:11:LEU:HD21	1:G:252:VAL:HG11	1.80	0.62
1:E:133:ARG:CG	1:E:133:ARG:HH11	2.06	0.62
1:G:18:THR:CG2	1:G:268:THR:HG22	2.29	0.62
1:G:91:ARG:NH2	1:G:203:ASN:HA	2.14	0.62
1:H:336:PRO:HG2	1:H:337:TYR:CD1	2.33	0.62
1:F:348:THR:OG1	1:F:406:GLU:HB3	1.99	0.62
1:G:68:HIS:O	1:G:492:ASN:ND2	2.32	0.62
1:H:194:ASN:HD22	1:H:199:LYS:HB3	1.63	0.62
1:G:393:GLN:HA	1:G:393:GLN:OE1	1.99	0.62
1:F:353:ASP:HB3	1:F:403:PRO:HB2	1.81	0.62
1:F:326:TYR:H	1:F:374:VAL:HG13	1.65	0.62
1:B:332:SER:CA	1:B:339:GLN:HE21	2.05	0.62
1:F:125:MET:HG2	1:F:188:LEU:HD13	1.80	0.62
1:G:254:LEU:HG	1:G:258:THR:CG2	2.30	0.62
1:A:398:THR:HB	1:A:400:MET:CG	2.29	0.62
1:A:19:GLY:N	1:A:268:THR:HG21	2.14	0.62
1:A:301:GLY:HA3	1:A:409:SER:HB3	1.81	0.62
1:F:22:ALA:HA	1:F:469:VAL:HG22	1.80	0.62
1:H:103:PRO:HB2	1:H:109:ASN:ND2	2.14	0.62
1:B:398:THR:CG2	1:B:400:MET:HG2	2.30	0.62
1:C:398:THR:O	1:C:398:THR:CG2	2.47	0.62
1:G:395:LEU:HD23	1:G:400:MET:HG3	1.82	0.62
1:E:271:VAL:HG13	1:E:287:THR:HG22	1.81	0.62
1:G:430:LEU:HD12	1:G:452:ARG:HE	1.65	0.62
1:A:309:ARG:HG3	1:A:310:ILE:HG13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:PRO:O	1:B:109:ASN:ND2	2.31	0.62
1:B:308:GLU:CD	1:B:308:GLU:H	2.03	0.62
1:E:25:ARG:HG2	1:E:469:VAL:HB	1.81	0.62
1:H:69:TYR:OH	1:H:487:VAL:HB	1.99	0.62
1:D:422:PRO:HA	1:D:426:ARG:HD3	1.82	0.62
1:A:142:PHE:O	1:A:146:ILE:HG13	1.98	0.62
1:G:336:PRO:HG2	1:G:337:TYR:CD1	2.35	0.62
1:F:17:PRO:O	1:F:462:PHE:HA	1.99	0.62
1:G:482:ASN:HB2	1:G:483:TYR:CE2	2.35	0.62
1:C:38:ASP:OD2	1:C:40:ASN:HB2	2.00	0.62
1:H:143:ASP:HA	1:H:146:ILE:HD12	1.82	0.62
1:E:440:LYS:HB2	1:E:442:ILE:HD12	1.82	0.62
1:C:490:ARG:NH2	1:G:483:TYR:OH	2.27	0.61
1:H:154:ILE:HD12	1:H:154:ILE:H	1.63	0.61
1:C:91:ARG:NH1	1:C:205:GLY:HA3	2.15	0.61
1:G:326:TYR:HE2	1:G:375:SER:N	1.98	0.61
1:A:125:MET:HE3	1:A:186:PRO:HB2	1.81	0.61
1:F:402:LYS:O	1:F:405:ASP:HB2	2.00	0.61
1:E:178:TRP:CB	1:E:454:GLU:HG3	2.30	0.61
1:B:271:VAL:HG12	1:B:448:PHE:O	2.00	0.61
1:F:367:TYR:CE1	1:F:408:VAL:HG21	2.35	0.61
1:G:323:CYS:HB2	1:G:325:PHE:CZ	2.35	0.61
1:F:115:LYS:O	1:F:119:VAL:HG23	1.99	0.61
1:A:108:ASN:N	1:A:108:ASN:OD1	2.20	0.61
1:E:461:SER:HA	1:E:464:LEU:CD1	2.24	0.61
1:A:107:GLN:O	1:A:110:ILE:HG13	2.00	0.61
1:H:432:GLN:O	1:H:436:LYS:HG2	2.00	0.61
1:B:296:HIS:CE1	1:B:382:VAL:HG21	2.34	0.61
1:C:296:HIS:CE1	1:C:382:VAL:HG21	2.36	0.61
1:G:222:TRP:HE3	1:G:222:TRP:HA	1.65	0.61
1:G:268:THR:HA	1:G:445:ARG:O	1.99	0.61
1:H:443:TRP:HB3	1:H:445:ARG:HE	1.65	0.61
1:B:125:MET:HE3	1:B:186:PRO:HB2	1.82	0.61
1:H:58:TYR:CE2	1:H:299:GLY:HA3	2.36	0.61
1:E:178:TRP:CE3	1:E:179:LEU:HD22	2.36	0.61
1:H:212:PHE:CD2	1:H:213:PRO:HD2	2.35	0.61
1:C:336:PRO:HG2	1:C:337:TYR:CE1	2.34	0.61
1:G:367:TYR:HD1	1:G:408:VAL:HG21	1.65	0.61
1:G:47:ALA:CB	1:G:222:TRP:HE1	2.11	0.61
1:E:169:VAL:HG23	1:E:170:PRO:O	2.01	0.61
1:G:60:VAL:HG12	1:G:60:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:VAL:HG13	1:F:287:THR:HG22	1.83	0.61
1:F:147:VAL:HG22	1:F:160:ARG:HH21	1.65	0.61
1:A:40:ASN:O	1:A:236:PHE:HB3	2.01	0.61
1:H:58:TYR:HD2	1:H:411:TYR:HD2	1.49	0.61
1:C:271:VAL:HA	1:C:274:LEU:HB2	1.82	0.61
1:G:57:LEU:CD1	1:G:338:ASN:HA	2.30	0.61
1:H:70:LYS:HE2	1:H:496:ARG:NH1	2.16	0.61
1:A:108:ASN:ND2	1:A:201:ALA:HB3	2.15	0.61
1:C:468:ALA:O	1:C:472:ILE:HG13	2.01	0.61
1:H:430:LEU:HD12	1:H:452:ARG:HE	1.64	0.61
1:F:118:GLN:OE1	1:F:195:VAL:HG13	2.00	0.61
1:B:60:VAL:O	1:B:63:HIS:NE2	2.34	0.61
1:G:222:TRP:HA	1:G:222:TRP:CE3	2.34	0.61
1:G:443:TRP:HB3	1:G:445:ARG:HE	1.66	0.61
1:G:492:ASN:ND2	1:G:492:ASN:N	2.49	0.61
1:H:446:GLY:N	1:H:450:SER:H	1.99	0.61
1:C:175:GLN:NE2	1:C:178:TRP:HD1	1.98	0.61
1:E:91:ARG:HG3	1:E:315:TRP:CH2	2.35	0.61
1:F:437:LEU:HB3	1:F:442:ILE:HB	1.81	0.61
1:D:58:TYR:HA	1:D:331:PHE:HE2	1.66	0.61
1:E:91:ARG:CD	1:E:207:ASN:HB2	2.31	0.61
1:F:178:TRP:CB	1:F:454:GLU:HG3	2.30	0.61
1:H:359:SER:HB3	1:H:363:LYS:CE	2.31	0.61
1:G:297:VAL:HB	1:G:415:PHE:HE2	1.64	0.61
1:B:144:GLU:O	1:B:148:ARG:HG3	2.00	0.61
1:G:69:TYR:OH	1:G:487:VAL:HB	2.01	0.61
1:H:445:ARG:NH1	1:H:481:LEU:HD22	2.16	0.61
1:C:178:TRP:HB2	1:C:454:GLU:CG	2.30	0.61
1:H:25:ARG:HD3	1:H:470:ASP:OD1	2.01	0.61
1:B:338:ASN:N	1:B:338:ASN:OD1	2.34	0.61
1:D:232:GLU:CD	1:D:232:GLU:H	2.04	0.61
1:G:115:LYS:O	1:G:118:GLN:HB2	2.01	0.60
1:H:150:MET:CG	1:H:154:ILE:HB	2.30	0.60
1:E:207:ASN:ND2	3:E:602:GDU:O4'	2.33	0.60
1:E:125:MET:HG2	1:E:188:LEU:HD13	1.82	0.60
1:C:60:VAL:O	1:C:63:HIS:NE2	2.34	0.60
1:A:398:THR:HB	1:A:400:MET:HG3	1.82	0.60
1:G:457:ASN:HB3	1:G:459:ASP:OD1	2.00	0.60
1:F:69:TYR:CZ	1:F:463:MET:HG3	2.36	0.60
1:G:478:GLU:HB2	1:G:481:LEU:HB3	1.83	0.60
1:C:91:ARG:NH2	1:C:204:TRP:O	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:124:GLY:C	1:G:151:GLY:HA3	2.20	0.60
1:D:245:VAL:HG22	1:D:252:VAL:HG23	1.81	0.60
1:G:338:ASN:HB2	1:G:339:GLN:HE22	1.66	0.60
1:D:108:ASN:ND2	1:D:201:ALA:HB3	2.16	0.60
1:E:6:ILE:HG22	1:E:260:ILE:HG23	1.82	0.60
1:F:145:TRP:CH2	1:F:183:VAL:HG21	2.36	0.60
1:E:145:TRP:CH2	1:E:183:VAL:HG21	2.36	0.60
1:B:170:PRO:HG2	1:B:173:LYS:HG3	1.83	0.60
1:C:251:THR:HA	1:C:260:ILE:O	2.01	0.60
1:D:163:ASN:HA	1:D:166:VAL:HG12	1.83	0.60
1:F:64:VAL:HB	3:F:602:GDU:O6'	2.02	0.60
1:F:9:ASP:O	1:F:263:LYS:HB2	2.02	0.60
1:D:176:CYS:O	1:D:179:LEU:HD12	2.01	0.60
1:E:183:VAL:HG11	3:E:602:GDU:O2	2.02	0.60
1:G:336:PRO:HG2	1:G:337:TYR:CE1	2.36	0.60
1:D:107:GLN:O	1:D:110:ILE:HG13	2.01	0.60
1:E:122:ILE:HG23	1:E:126:ILE:HD11	1.83	0.60
1:H:203:ASN:O	1:H:204:TRP:HB2	2.01	0.60
1:F:265:LEU:HD23	1:F:442:ILE:HG12	1.82	0.60
1:B:411:TYR:C	1:B:411:TYR:CD2	2.75	0.60
1:E:346:LEU:HD12	1:E:367:TYR:CZ	2.37	0.60
1:D:18:THR:OG1	1:D:461:SER:HB3	2.01	0.60
2:F:601:FAD:O4	3:F:602:GDU:H2'	2.02	0.60
1:F:322:ASN:ND2	1:F:398:THR:HG22	2.16	0.60
1:G:168:ALA:HB1	1:G:377:SER:OG	2.02	0.60
1:H:47:ALA:CB	1:H:222:TRP:HE1	2.09	0.60
1:C:504:PHE:HA	1:C:507:SER:HB3	1.84	0.60
1:H:162:TYR:CZ	1:H:166:VAL:HG11	2.36	0.60
1:G:325:PHE:CD2	1:G:372:LEU:HD22	2.37	0.60
1:C:411:TYR:CD2	1:C:411:TYR:C	2.74	0.60
1:D:411:TYR:CD2	1:D:411:TYR:C	2.75	0.60
1:H:457:ASN:HB3	1:H:459:ASP:OD1	2.02	0.60
1:D:57:LEU:HD22	1:D:338:ASN:HA	1.84	0.60
1:F:122:ILE:HG22	1:F:123:ASP:N	2.17	0.60
1:H:309:ARG:HG2	1:H:310:ILE:HD12	1.84	0.60
1:G:53:PRO:HB2	1:G:54:GLU:OE2	2.02	0.60
1:C:125:MET:HE3	1:C:186:PRO:HB2	1.84	0.60
1:B:91:ARG:NH1	1:B:205:GLY:HA3	2.17	0.60
1:G:274:LEU:O	1:G:278:MET:HG2	2.02	0.60
1:H:250:LYS:HB3	1:H:262:TYR:O	2.02	0.60
1:F:471:ASN:ND2	1:F:476:ALA:O	2.25	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:TRP:CD2	1:F:174:MET:HE1	2.36	0.59
1:G:91:ARG:N	1:G:208:ALA:O	2.30	0.59
1:A:429:ALA:O	1:A:433:ILE:HD12	2.03	0.59
1:E:322:ASN:ND2	1:E:398:THR:HG22	2.18	0.59
1:H:395:LEU:HD23	1:H:400:MET:HG3	1.85	0.59
1:F:91:ARG:CD	1:F:207:ASN:HB2	2.32	0.59
1:H:204:TRP:HA	1:H:204:TRP:HE3	1.66	0.59
1:A:271:VAL:HA	1:A:274:LEU:HB2	1.83	0.59
1:G:248:ASN:N	1:G:248:ASN:OD1	2.34	0.59
1:A:336:PRO:HG2	1:A:337:TYR:CD1	2.37	0.59
1:C:242:VAL:HG23	2:C:601:FAD:N1A	2.16	0.59
1:B:301:GLY:HA3	1:B:409:SER:HB3	1.85	0.59
1:B:245:VAL:HG22	1:B:252:VAL:HG23	1.84	0.59
1:G:170:PRO:HD2	1:G:379:MET:SD	2.42	0.59
1:E:402:LYS:O	1:E:405:ASP:HB2	2.02	0.59
1:D:143:ASP:HA	1:D:146:ILE:HD12	1.84	0.59
1:H:303:ARG:NH2	1:H:346:LEU:O	2.35	0.59
1:D:336:PRO:HG2	1:D:337:TYR:CE1	2.36	0.59
1:D:43:PRO:HG2	1:D:223:ILE:HD13	1.84	0.59
1:H:285:GLY:O	1:H:288:LYS:HB2	2.02	0.59
1:C:455:VAL:CG1	1:C:464:LEU:HD11	2.32	0.59
1:E:94:TYR:HB2	1:E:316:LEU:HD22	1.82	0.59
1:F:160:ARG:N	1:F:161:PRO:HD2	2.18	0.59
1:F:38:ASP:HB3	1:F:236:PHE:HD1	1.67	0.59
1:B:107:GLN:O	1:B:110:ILE:HG13	2.01	0.59
1:G:443:TRP:HA	1:G:445:ARG:HH21	1.68	0.59
1:H:70:LYS:HE2	1:H:496:ARG:HH12	1.67	0.59
1:B:419:TYR:CE1	2:B:601:FAD:HM73	2.36	0.59
1:G:353:ASP:HB3	1:G:403:PRO:CB	2.32	0.59
1:F:437:LEU:O	1:F:442:ILE:N	2.35	0.59
1:F:350:GLN:O	1:F:407:ILE:HB	2.02	0.59
1:C:346:LEU:HD23	1:C:347:PRO:HD2	1.85	0.59
1:F:154:ILE:CD1	1:F:154:ILE:H	1.99	0.59
1:H:445:ARG:HA	1:H:450:SER:CB	2.32	0.59
1:B:422:PRO:HA	1:B:426:ARG:HD3	1.84	0.59
1:F:69:TYR:CE1	1:F:463:MET:HG3	2.37	0.59
1:B:54:GLU:HB3	1:B:346:LEU:HD11	1.84	0.59
1:A:32:PRO:HB3	1:E:504:PHE:CD2	2.37	0.59
1:H:383:ASN:HD22	1:H:386:THR:HG23	1.67	0.59
1:G:471:ASN:HA	1:G:476:ALA:H	1.68	0.59
1:G:25:ARG:HA	1:G:28:GLN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:LYS:HB3	1:G:262:TYR:O	2.02	0.59
1:B:463:MET:O	1:B:467:GLU:HG3	2.03	0.59
1:B:57:LEU:H	1:B:57:LEU:HD13	1.67	0.59
1:F:224:ALA:O	1:F:228:THR:HG23	2.03	0.59
1:G:492:ASN:HD22	1:G:492:ASN:N	2.00	0.59
1:A:109:ASN:OD1	1:A:200:THR:HG22	2.03	0.59
1:H:142:PHE:HA	1:H:176:CYS:HB3	1.85	0.59
1:F:69:TYR:HB2	1:F:72:PHE:HB3	1.85	0.59
1:A:411:TYR:CD2	1:A:411:TYR:C	2.76	0.59
1:G:23:ALA:HA	1:G:26:LEU:HD12	1.84	0.59
1:B:429:ALA:O	1:B:433:ILE:HD12	2.03	0.59
1:C:308:GLU:H	1:C:308:GLU:CD	2.06	0.59
1:A:126:ILE:HD12	1:G:189:LYS:HG2	1.84	0.58
1:F:178:TRP:CE3	1:F:179:LEU:HD22	2.38	0.58
1:C:170:PRO:HG2	1:C:173:LYS:HG3	1.84	0.58
1:B:383:ASN:O	1:B:387:ILE:HB	2.03	0.58
1:H:348:THR:HG21	1:H:406:GLU:HG2	1.83	0.58
1:G:58:TYR:HE1	1:G:369:SER:OG	1.85	0.58
1:F:346:LEU:HD12	1:F:367:TYR:CZ	2.38	0.58
1:F:70:LYS:HB3	1:F:496:ARG:HH12	1.67	0.58
1:G:464:LEU:HG	1:G:480:THR:HB	1.85	0.58
1:B:309:ARG:HG3	1:B:310:ILE:HG13	1.86	0.58
1:F:502:GLN:O	1:F:506:LYS:HD3	2.03	0.58
1:G:462:PHE:O	1:G:466:VAL:HG23	2.03	0.58
1:H:341:GLU:HG3	1:H:343:SER:H	1.68	0.58
1:E:97:CYS:SG	1:E:98:GLN:HG3	2.43	0.58
1:A:95:VAL:HG23	1:A:102:VAL:O	2.02	0.58
1:G:107:GLN:H	1:G:107:GLN:CD	2.06	0.58
1:G:411:TYR:CD1	1:G:411:TYR:C	2.75	0.58
1:A:57:LEU:HD22	1:A:338:ASN:HA	1.85	0.58
1:A:197:LEU:CD2	1:G:115:LYS:HD3	2.33	0.58
1:G:197:LEU:O	1:G:199:LYS:N	2.37	0.58
1:A:178:TRP:HB2	1:A:454:GLU:CG	2.32	0.58
1:D:16:GLY:H	2:D:601:FAD:H4B	1.68	0.58
1:D:457:ASN:O	1:D:460:HIS:HB2	2.03	0.58
1:E:303:ARG:HH21	1:E:363:LYS:CB	2.17	0.58
1:E:184:ALA:HB2	1:E:204:TRP:CD2	2.38	0.58
1:D:338:ASN:N	1:D:338:ASN:OD1	2.36	0.58
1:H:341:GLU:HG3	1:H:342:ALA:N	2.18	0.58
1:B:352:ALA:HB3	1:B:403:PRO:HA	1.86	0.58
1:H:44:GLY:HA3	1:H:222:TRP:CD1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:ARG:HD2	3:C:602:GDU:O1A	2.04	0.58
1:C:453:TYR:OH	3:C:602:GDU:O2B	2.22	0.58
3:C:602:GDU:O1B	3:C:602:GDU:H5'2	2.04	0.58
1:E:207:ASN:HB3	1:E:315:TRP:CH2	2.39	0.58
1:C:93:SER:HB2	1:C:104:TYR:HB3	1.83	0.58
1:B:504:PHE:HA	1:B:507:SER:HB3	1.85	0.58
1:G:367:TYR:HE1	1:G:408:VAL:HG11	1.68	0.58
1:H:11:LEU:O	1:H:265:LEU:HD12	2.04	0.58
1:A:303:ARG:NH1	1:A:348:THR:OG1	2.37	0.58
1:E:163:ASN:HA	1:E:166:VAL:HG13	1.85	0.58
1:H:103:PRO:CB	1:H:202:GLY:HA2	2.33	0.58
1:F:94:TYR:HB2	1:F:316:LEU:HD22	1.84	0.58
1:C:103:PRO:CB	1:C:109:ASN:ND2	2.66	0.58
1:C:16:GLY:H	2:C:601:FAD:H52A	1.68	0.58
1:C:232:GLU:H	1:C:232:GLU:CD	2.07	0.58
1:H:418:GLY:C	1:H:419:TYR:CD1	2.75	0.58
1:H:124:GLY:C	1:H:151:GLY:HA3	2.22	0.58
1:H:44:GLY:CA	1:H:222:TRP:CD1	2.86	0.58
1:C:113:LEU:O	1:C:118:GLN:NE2	2.29	0.58
1:E:160:ARG:N	1:E:161:PRO:HD2	2.18	0.58
1:H:331:PHE:CD2	1:H:338:ASN:HB3	2.39	0.58
1:A:416:ASP:HB2	1:F:281:GLN:NE2	2.19	0.58
1:H:433:ILE:O	1:H:436:LYS:HB2	2.03	0.58
1:H:85:ASP:HA	1:H:214:ALA:HB2	1.86	0.58
1:C:301:GLY:HA3	1:C:409:SER:HB3	1.85	0.58
1:C:245:VAL:HG22	1:C:252:VAL:HG23	1.85	0.58
1:E:248:ASN:N	1:E:248:ASN:OD1	2.37	0.58
1:E:26:LEU:HD13	1:E:34:TRP:HB2	1.86	0.58
1:D:91:ARG:HD3	1:D:207:ASN:CB	2.34	0.58
1:C:136:ASN:N	1:C:136:ASN:OD1	2.35	0.58
1:C:54:GLU:HB3	1:C:346:LEU:HD11	1.86	0.58
1:B:20:LEU:N	1:B:20:LEU:HD23	2.19	0.58
1:D:60:VAL:O	1:D:63:HIS:NE2	2.37	0.58
1:C:455:VAL:HG21	1:C:480:THR:O	2.04	0.58
1:E:103:PRO:HB2	1:E:109:ASN:OD1	2.04	0.58
1:D:325:PHE:HA	1:D:374:VAL:HG22	1.85	0.58
1:C:411:TYR:HD2	1:C:411:TYR:C	2.07	0.58
1:C:499:ASP:O	1:C:503:VAL:HG23	2.04	0.58
1:C:11:LEU:O	1:C:265:LEU:HD12	2.04	0.58
1:G:446:GLY:N	1:G:450:SER:H	2.01	0.57
2:E:601:FAD:O4	3:E:602:GDU:H2'	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:455:VAL:CG1	1:D:464:LEU:HD11	2.33	0.57
1:A:350:GLN:NE2	1:A:354:GLY:HA2	2.16	0.57
1:D:466:VAL:HG12	1:D:495:ARG:NH1	2.19	0.57
1:A:143:ASP:O	1:A:147:VAL:HG23	2.04	0.57
1:E:351:LEU:HA	1:E:405:ASP:O	2.04	0.57
1:B:303:ARG:HH21	1:B:363:LYS:C	2.06	0.57
1:A:170:PRO:HG2	1:A:173:LYS:HG3	1.86	0.57
1:E:64:VAL:HG22	1:E:210:PHE:CE1	2.39	0.57
1:A:47:ALA:HB1	1:A:222:TRP:HE1	1.69	0.57
1:H:149:MET:SD	1:H:184:ALA:CA	2.86	0.57
1:H:249:ASN:N	1:H:249:ASN:OD1	2.37	0.57
1:C:463:MET:O	1:C:467:GLU:HG3	2.04	0.57
1:B:411:TYR:C	1:B:411:TYR:HD2	2.07	0.57
1:H:89:HIS:HB2	1:H:210:PHE:CE2	2.39	0.57
1:D:309:ARG:HG3	1:D:310:ILE:HG13	1.85	0.57
1:B:163:ASN:HA	1:B:166:VAL:HG12	1.86	0.57
1:H:189:LYS:O	1:H:193:THR:OG1	2.21	0.57
1:G:383:ASN:HD22	1:G:386:THR:HG23	1.69	0.57
1:G:285:GLY:O	1:G:288:LYS:HB2	2.05	0.57
1:G:467:GLU:OE1	1:G:480:THR:N	2.24	0.57
1:A:271:VAL:HG12	1:A:448:PHE:O	2.04	0.57
1:C:309:ARG:HG3	1:C:310:ILE:HG13	1.87	0.57
1:H:248:ASN:OD1	1:H:248:ASN:N	2.37	0.57
1:F:445:ARG:CZ	1:F:481:LEU:HD22	2.34	0.57
1:E:10:VAL:HG22	1:E:264:LYS:HG3	1.86	0.57
1:H:492:ASN:HD22	1:H:492:ASN:H	1.52	0.57
1:H:222:TRP:HA	1:H:222:TRP:CE3	2.39	0.57
1:C:107:GLN:O	1:C:110:ILE:HG13	2.04	0.57
1:D:142:PHE:O	1:D:146:ILE:HG13	2.05	0.57
1:E:263:LYS:N	1:E:263:LYS:HD2	2.19	0.57
1:E:69:TYR:CZ	1:E:463:MET:HG3	2.39	0.57
1:H:158:PHE:HE1	1:H:162:TYR:CG	2.22	0.57
1:B:47:ALA:HB1	1:B:222:TRP:NE1	2.19	0.57
1:E:303:ARG:NH2	1:E:363:LYS:CG	2.67	0.57
1:H:25:ARG:HH11	1:H:470:ASP:CG	2.07	0.57
1:D:483:TYR:OH	1:H:490:ARG:NH2	2.22	0.57
1:H:344:LYS:O	1:H:367:TYR:OH	2.22	0.57
1:F:154:ILE:HD13	1:F:154:ILE:N	2.12	0.57
1:B:175:GLN:NE2	1:B:178:TRP:HD1	2.03	0.57
1:E:167:TRP:CE3	1:E:421:THR:HG22	2.39	0.57
1:C:196:ILE:HG21	1:E:119:VAL:HG23	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:28:GLN:HG2	1:H:497:LEU:O	2.05	0.57
1:B:109:ASN:OD1	1:B:200:THR:HG22	2.04	0.57
1:C:57:LEU:HD13	1:C:338:ASN:O	2.03	0.57
1:A:338:ASN:N	1:A:338:ASN:OD1	2.37	0.57
1:D:199:LYS:HD2	1:D:200:THR:O	2.04	0.57
1:F:368:TRP:CZ3	1:F:370:ILE:HD11	2.40	0.57
1:A:20:LEU:N	1:A:20:LEU:HD23	2.19	0.57
1:E:71:TYR:CD2	1:E:496:ARG:HA	2.39	0.57
1:F:167:TRP:CE3	1:F:421:THR:HG22	2.39	0.57
1:F:150:MET:HG3	1:F:154:ILE:HB	1.85	0.57
1:H:17:PRO:HD2	2:H:601:FAD:O5'	2.03	0.57
1:D:458:GLN:CG	2:D:601:FAD:H2'	2.34	0.57
1:H:25:ARG:NH1	1:H:470:ASP:OD1	2.25	0.57
1:H:91:ARG:N	1:H:208:ALA:O	2.30	0.57
1:F:19:GLY:O	1:F:22:ALA:HB3	2.05	0.57
1:F:26:LEU:HD13	1:F:34:TRP:HB2	1.87	0.57
1:G:292:TYR:CE1	1:G:417:HIS:ND1	2.70	0.57
1:A:183:VAL:HG13	3:A:602:GDU:C2	2.32	0.57
1:E:143:ASP:O	1:E:147:VAL:HG23	2.04	0.57
1:G:103:PRO:CB	1:G:202:GLY:HA3	2.34	0.57
1:C:47:ALA:HB1	1:C:222:TRP:NE1	2.19	0.57
1:G:11:LEU:O	1:G:265:LEU:HD12	2.05	0.57
1:C:58:TYR:HA	1:C:331:PHE:CE2	2.40	0.57
1:A:306:ARG:CZ	1:A:311:GLY:HA2	2.34	0.57
1:G:438:GLN:HA	1:G:442:ILE:O	2.05	0.57
1:D:429:ALA:O	1:D:433:ILE:HD12	2.04	0.57
1:F:72:PHE:CZ	1:F:76:LEU:HD11	2.40	0.57
1:F:6:ILE:HG22	1:F:260:ILE:HG23	1.87	0.57
1:E:502:GLN:O	1:E:506:LYS:HD3	2.03	0.57
1:B:136:ASN:OD1	1:B:136:ASN:N	2.32	0.57
1:B:136:ASN:OD1	1:B:137:THR:HG23	2.05	0.57
1:E:323:CYS:HB2	1:E:324:PRO:HD2	1.86	0.57
1:A:175:GLN:NE2	1:A:178:TRP:HD1	2.03	0.57
1:F:467:GLU:CG	1:F:495:ARG:HH12	2.12	0.56
1:F:9:ASP:N	1:F:33:SER:OG	2.28	0.56
1:E:325:PHE:HA	1:E:374:VAL:CG1	2.35	0.56
1:H:455:VAL:O	1:H:460:HIS:CB	2.49	0.56
1:E:104:TYR:HE1	3:E:602:GDU:C4	2.18	0.56
1:H:58:TYR:HE1	1:H:369:SER:OG	1.88	0.56
1:D:344:LYS:HD2	1:D:345:LYS:N	2.20	0.56
1:B:456:GLY:O	2:B:601:FAD:O3'	2.22	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:458:GLN:HG2	2:G:601:FAD:H2'	1.86	0.56
1:E:326:TYR:OH	1:E:373:GLU:OE2	2.23	0.56
1:H:480:THR:HA	1:H:487:VAL:HG21	1.87	0.56
1:F:335:SER:HB3	1:F:338:ASN:OD1	2.05	0.56
1:H:162:TYR:O	1:H:165:LYS:N	2.37	0.56
1:G:162:TYR:O	1:G:165:LYS:N	2.38	0.56
1:B:455:VAL:CG1	1:B:464:LEU:HD11	2.35	0.56
1:H:411:TYR:CD1	1:H:411:TYR:C	2.77	0.56
1:H:58:TYR:HD2	1:H:411:TYR:CD2	2.22	0.56
1:H:141:THR:OG1	1:H:144:GLU:HB2	2.05	0.56
1:F:427:GLU:O	1:F:431:THR:HG23	2.05	0.56
1:H:462:PHE:O	1:H:466:VAL:HG23	2.05	0.56
1:A:411:TYR:HD2	1:A:411:TYR:C	2.08	0.56
1:H:13:ILE:HD12	1:H:265:LEU:HD11	1.88	0.56
1:B:163:ASN:HA	1:B:166:VAL:CG1	2.35	0.56
1:A:212:PHE:CG	1:A:213:PRO:HD2	2.40	0.56
1:D:125:MET:HE3	1:D:186:PRO:HB2	1.87	0.56
1:C:352:ALA:HB3	1:C:403:PRO:HA	1.87	0.56
1:A:388:LEU:O	1:A:392:ILE:HG13	2.04	0.56
1:A:134:VAL:O	1:A:134:VAL:CG1	2.53	0.56
1:A:163:ASN:HA	1:A:166:VAL:HG12	1.87	0.56
1:H:353:ASP:HB3	1:H:403:PRO:HB3	1.87	0.56
1:E:21:GLY:HA2	1:E:462:PHE:CE1	2.41	0.56
1:G:38:ASP:OD1	2:G:601:FAD:O3B	2.23	0.56
1:E:151:GLY:O	1:E:154:ILE:HG12	2.05	0.56
1:A:91:ARG:HD3	1:A:207:ASN:CB	2.34	0.56
1:B:395:LEU:HD22	1:B:400:MET:HE2	1.86	0.56
1:H:306:ARG:HH11	1:H:312:ASP:HA	1.68	0.56
1:G:402:LYS:HD3	1:G:405:ASP:OD2	2.04	0.56
1:F:169:VAL:HG23	1:F:170:PRO:O	2.05	0.56
1:B:466:VAL:HG12	1:B:495:ARG:NH1	2.20	0.56
1:B:183:VAL:CG2	3:B:602:GDU:H1D	2.24	0.56
1:C:422:PRO:HA	1:C:426:ARG:HD3	1.86	0.56
1:D:457:ASN:HA	2:D:601:FAD:H1'2	1.88	0.56
1:F:6:ILE:O	1:F:260:ILE:HA	2.05	0.56
1:B:139:PRO:HB2	1:B:176:CYS:SG	2.46	0.56
1:C:103:PRO:C	1:C:109:ASN:HD22	2.07	0.56
1:C:38:ASP:HA	2:C:601:FAD:H2A	1.87	0.56
1:A:433:ILE:O	1:A:436:LYS:HB2	2.05	0.56
1:D:144:GLU:O	1:D:148:ARG:HG3	2.05	0.56
1:A:64:VAL:HG13	1:A:210:PHE:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:GLU:CD	1:D:308:GLU:H	2.09	0.56
1:F:64:VAL:HG22	1:F:210:PHE:CE1	2.41	0.56
1:F:17:PRO:O	1:F:462:PHE:HD1	1.88	0.56
1:E:27:ASN:HB2	1:E:34:TRP:HZ2	1.70	0.56
1:G:204:TRP:HA	1:G:204:TRP:CE3	2.39	0.56
1:E:147:VAL:HG22	1:E:160:ARG:HH21	1.71	0.56
1:E:72:PHE:CZ	1:E:76:LEU:HD11	2.41	0.56
1:F:303:ARG:NH2	1:F:363:LYS:HB2	2.19	0.56
1:G:250:LYS:O	1:G:261:GLY:HA2	2.06	0.56
1:D:411:TYR:HD2	1:D:411:TYR:C	2.09	0.56
1:H:453:TYR:CD2	1:H:453:TYR:C	2.79	0.56
1:D:93:SER:HB2	1:D:104:TYR:HB3	1.88	0.56
1:F:101:TRP:HZ3	1:F:316:LEU:HD13	1.71	0.56
1:F:353:ASP:HB3	1:F:403:PRO:HB3	1.87	0.56
1:B:336:PRO:HG2	1:B:337:TYR:CE1	2.41	0.56
1:F:109:ASN:H	1:F:109:ASN:HD22	1.54	0.56
1:B:143:ASP:HA	1:B:146:ILE:HD12	1.87	0.56
1:E:460:HIS:O	1:E:463:MET:HB2	2.05	0.56
1:C:163:ASN:HA	1:C:166:VAL:CG1	2.35	0.56
1:A:143:ASP:HA	1:A:146:ILE:HD12	1.88	0.56
1:E:367:TYR:CE1	1:E:408:VAL:HG21	2.40	0.56
1:C:346:LEU:HD23	1:C:347:PRO:CD	2.36	0.56
1:F:270:ALA:HB3	1:F:273:PHE:CD2	2.41	0.56
1:B:18:THR:OG1	1:B:461:SER:HB3	2.05	0.56
1:C:160:ARG:N	1:C:161:PRO:HD2	2.21	0.56
1:E:424:LEU:HB2	1:E:425:GLU:OE1	2.06	0.56
1:F:163:ASN:HA	1:F:166:VAL:HG13	1.88	0.56
1:B:93:SER:HB2	1:B:104:TYR:HB3	1.86	0.56
1:A:398:THR:HG22	1:A:398:THR:O	2.05	0.56
1:B:504:PHE:HZ	1:F:264:LYS:CG	2.20	0.56
1:F:47:ALA:HB1	1:F:222:TRP:NE1	2.21	0.56
1:D:20:LEU:N	1:D:20:LEU:HD23	2.20	0.56
1:A:308:GLU:CD	1:A:308:GLU:H	2.09	0.56
1:F:63:HIS:CE1	2:F:601:FAD:C9A	2.89	0.55
1:G:272:ASP:OD1	1:G:272:ASP:N	2.38	0.55
1:A:105:PRO:O	1:A:109:ASN:ND2	2.38	0.55
1:E:69:TYR:CE1	1:E:463:MET:HG3	2.41	0.55
1:D:64:VAL:HG13	1:D:210:PHE:CD1	2.40	0.55
1:H:96:ARG:HA	1:H:100:GLN:O	2.05	0.55
1:A:352:ALA:HB3	1:A:403:PRO:HA	1.87	0.55
1:G:349:MET:SD	1:G:409:SER:HA	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:PRO:O	1:E:462:PHE:HD1	1.88	0.55
1:H:222:TRP:HE3	1:H:222:TRP:HA	1.71	0.55
1:A:38:ASP:OD1	2:A:601:FAD:H1B	2.06	0.55
1:G:96:ARG:HA	1:G:100:GLN:O	2.07	0.55
1:C:163:ASN:HA	1:C:166:VAL:HG12	1.87	0.55
1:B:480:THR:HA	1:B:487:VAL:HG11	1.88	0.55
1:H:383:ASN:ND2	1:H:386:THR:HG23	2.21	0.55
1:D:344:LYS:HD2	1:D:345:LYS:H	1.72	0.55
1:B:8:VAL:HG11	1:B:35:MET:HG2	1.88	0.55
1:E:230:PRO:CG	1:E:233:LYS:HD2	2.36	0.55
1:E:114:PRO:O	1:E:118:GLN:HG3	2.06	0.55
1:G:158:PHE:C	1:G:158:PHE:CD1	2.80	0.55
1:D:398:THR:HB	1:D:400:MET:HG3	1.89	0.55
1:D:398:THR:HB	1:D:400:MET:HG2	1.87	0.55
1:H:64:VAL:HG22	1:H:210:PHE:CD1	2.41	0.55
1:A:383:ASN:O	1:A:387:ILE:HB	2.06	0.55
1:E:27:ASN:OD1	1:E:27:ASN:C	2.44	0.55
1:E:26:LEU:HG	1:E:469:VAL:HG13	1.89	0.55
1:G:458:GLN:HA	2:G:601:FAD:O3'	2.07	0.55
1:D:91:ARG:NH2	1:D:204:TRP:O	2.32	0.55
1:D:242:VAL:HB	2:D:601:FAD:H62A	1.69	0.55
1:D:64:VAL:O	2:D:601:FAD:N3	2.37	0.55
1:H:25:ARG:HA	1:H:28:GLN:HB2	1.89	0.55
1:G:212:PHE:CG	1:G:213:PRO:HD2	2.41	0.55
1:D:27:ASN:OD1	1:D:230:PRO:HD2	2.07	0.55
1:E:116:GLU:HG2	1:E:117:GLU:N	2.20	0.55
1:F:116:GLU:HG2	1:F:117:GLU:N	2.19	0.55
1:B:468:ALA:O	1:B:472:ILE:HG13	2.06	0.55
1:B:16:GLY:HA3	2:B:601:FAD:O1A	2.06	0.55
1:C:494:GLU:OE2	1:G:477:VAL:HB	2.07	0.55
1:D:187:ASN:OD1	1:D:187:ASN:C	2.44	0.55
1:H:115:LYS:O	1:H:118:GLN:HB2	2.07	0.55
1:D:69:TYR:CD1	1:D:463:MET:HG3	2.41	0.55
1:C:338:ASN:OD1	1:C:338:ASN:N	2.40	0.55
1:A:87:TYR:HB3	1:A:89:HIS:CE1	2.42	0.55
1:H:478:GLU:HB2	1:H:481:LEU:HB3	1.88	0.55
1:F:332:SER:HA	1:F:339:GLN:HE21	1.71	0.55
1:G:346:LEU:CD2	1:G:347:PRO:HD2	2.35	0.55
1:B:455:VAL:HG21	1:B:480:THR:O	2.06	0.55
1:B:69:TYR:CD1	1:B:463:MET:HG3	2.42	0.55
1:A:11:LEU:O	1:A:265:LEU:HD12	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:THR:HA	1:B:260:ILE:O	2.06	0.55
1:G:453:TYR:CD2	1:G:453:TYR:C	2.79	0.55
1:C:134:VAL:O	1:C:134:VAL:CG1	2.54	0.55
1:G:358:GLN:OE1	1:G:358:GLN:HA	2.06	0.55
1:H:458:GLN:HG3	2:H:601:FAD:O2	2.07	0.55
1:A:38:ASP:OD2	1:A:40:ASN:HB2	2.06	0.55
1:E:68:HIS:CE1	1:E:460:HIS:NE2	2.75	0.55
1:E:136:ASN:OD1	1:E:137:THR:HG23	2.07	0.55
1:B:306:ARG:CZ	1:B:311:GLY:HA2	2.37	0.55
1:C:20:LEU:N	1:C:20:LEU:HD23	2.21	0.55
1:D:251:THR:HA	1:D:260:ILE:O	2.06	0.55
1:G:484:PRO:HA	1:G:487:VAL:HG22	1.89	0.55
1:A:107:GLN:NE2	3:A:602:GDU:O4	2.40	0.55
1:H:79:ALA:HB2	1:H:225:VAL:CG2	2.36	0.55
1:G:158:PHE:C	1:G:158:PHE:HD1	2.10	0.55
1:H:207:ASN:OD1	1:H:207:ASN:C	2.45	0.55
1:F:147:VAL:CG2	1:F:160:ARG:HH21	2.20	0.55
1:H:464:LEU:HG	1:H:480:THR:HB	1.88	0.55
1:A:422:PRO:HA	1:A:426:ARG:HD3	1.88	0.55
1:E:179:LEU:HD23	1:E:179:LEU:H	1.70	0.55
1:G:103:PRO:HB3	1:G:202:GLY:HA3	1.89	0.55
1:E:383:ASN:ND2	1:E:386:THR:HG23	2.22	0.55
1:A:251:THR:HA	1:A:260:ILE:O	2.07	0.55
1:F:219:GLY:O	1:F:223:ILE:HG12	2.07	0.55
1:G:232:GLU:N	1:G:232:GLU:OE1	2.25	0.55
1:F:150:MET:O	1:F:154:ILE:HG13	2.07	0.54
1:H:299:GLY:HA2	1:H:371:MET:HA	1.89	0.54
1:E:110:ILE:HG23	1:E:195:VAL:HG22	1.89	0.54
1:C:143:ASP:HA	1:C:146:ILE:HD12	1.89	0.54
1:H:11:LEU:HD21	1:H:252:VAL:HG11	1.87	0.54
1:B:160:ARG:N	1:B:161:PRO:HD2	2.23	0.54
1:H:170:PRO:HD2	1:H:379:MET:SD	2.47	0.54
1:F:457:ASN:HB3	2:F:601:FAD:O2	2.06	0.54
1:E:26:LEU:HD22	1:E:34:TRP:HB3	1.90	0.54
1:B:62:GLY:O	3:B:602:GDU:H6'1	2.07	0.54
1:A:46:LEU:N	2:A:601:FAD:O1A	2.35	0.54
1:C:457:ASN:O	1:C:460:HIS:HB2	2.08	0.54
1:E:376:GLU:HB2	1:E:382:VAL:CG1	2.37	0.54
1:F:298:ILE:CD1	1:F:388:LEU:HD13	2.38	0.54
1:E:19:GLY:CA	1:E:268:THR:HG21	2.37	0.54
1:C:453:TYR:OH	3:C:602:GDU:PB	2.64	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:494:GLU:HG2	1:G:477:VAL:CA	2.32	0.54
1:C:125:MET:CE	1:C:186:PRO:HB2	2.38	0.54
1:C:455:VAL:HG13	1:C:455:VAL:O	2.05	0.54
1:A:144:GLU:O	1:A:148:ARG:HG3	2.07	0.54
1:D:17:PRO:HD2	2:D:601:FAD:O5'	2.06	0.54
1:H:8:VAL:O	1:H:262:TYR:HA	2.07	0.54
1:B:155:ALA:O	1:B:160:ARG:HG3	2.07	0.54
1:C:95:VAL:HG23	1:C:102:VAL:O	2.07	0.54
1:G:143:ASP:O	1:G:147:VAL:HG23	2.08	0.54
1:C:336:PRO:HG2	1:C:337:TYR:CD1	2.42	0.54
1:C:57:LEU:HD22	1:C:338:ASN:HA	1.89	0.54
1:G:89:HIS:HB2	1:G:210:PHE:CE2	2.42	0.54
1:A:468:ALA:O	1:A:472:ILE:HG13	2.06	0.54
1:G:418:GLY:C	1:G:419:TYR:CD1	2.79	0.54
1:C:182:ARG:HD2	3:C:602:GDU:O2A	2.08	0.54
1:B:178:TRP:HB2	1:B:454:GLU:CG	2.33	0.54
1:H:337:TYR:N	1:H:337:TYR:CD1	2.75	0.54
1:G:411:TYR:CD1	1:G:412:HIS:N	2.69	0.54
1:G:303:ARG:NH1	1:G:348:THR:OG1	2.26	0.54
1:F:303:ARG:NH2	1:F:363:LYS:CB	2.71	0.54
1:F:204:TRP:CE3	1:F:205:GLY:HA2	2.43	0.54
1:C:57:LEU:H	1:C:57:LEU:HD13	1.73	0.54
1:F:25:ARG:HG2	1:F:469:VAL:HB	1.90	0.54
1:G:411:TYR:HD1	1:G:411:TYR:C	2.10	0.54
1:G:29:ILE:HG22	1:G:31:GLY:N	2.22	0.54
1:A:455:VAL:HG13	1:A:455:VAL:O	2.08	0.54
1:G:341:GLU:HG3	1:G:342:ALA:N	2.21	0.54
1:B:457:ASN:O	1:B:460:HIS:HB2	2.08	0.54
1:G:434:LEU:HB2	1:G:435:PRO:HD3	1.90	0.54
2:F:601:FAD:C2'	2:F:601:FAD:H9	2.38	0.54
1:C:142:PHE:O	1:C:146:ILE:HG13	2.07	0.54
1:C:60:VAL:O	1:C:63:HIS:CD2	2.61	0.54
1:D:168:ALA:CB	1:D:377:SER:HB3	2.38	0.54
1:C:64:VAL:HG13	1:C:210:PHE:CD1	2.42	0.54
1:A:446:GLY:H	1:A:450:SER:HB2	1.72	0.54
1:H:23:ALA:HA	1:H:26:LEU:HD12	1.89	0.54
1:F:248:ASN:N	1:F:248:ASN:OD1	2.40	0.54
1:F:309:ARG:HD3	1:F:309:ARG:H	1.73	0.54
1:D:143:ASP:O	1:D:147:VAL:HG23	2.08	0.54
1:C:175:GLN:HE21	1:C:178:TRP:HD1	1.56	0.54
1:G:58:TYR:HD2	1:G:411:TYR:CD2	2.25	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:207:ASN:HB3	1:F:315:TRP:CH2	2.42	0.54
1:H:426:ARG:O	1:H:430:LEU:HG	2.08	0.54
1:A:504:PHE:HA	1:A:507:SER:HB3	1.88	0.54
1:D:383:ASN:O	1:D:387:ILE:HB	2.07	0.54
1:G:480:THR:HA	1:G:487:VAL:HG21	1.90	0.54
1:H:54:GLU:HB3	1:H:346:LEU:CD1	2.38	0.54
1:H:402:LYS:HD3	1:H:405:ASP:OD2	2.07	0.54
1:D:136:ASN:N	1:D:136:ASN:OD1	2.34	0.54
1:A:433:ILE:HG22	1:A:434:LEU:N	2.23	0.54
1:B:344:LYS:HD2	1:B:345:LYS:N	2.23	0.54
1:C:18:THR:OG1	1:C:461:SER:HB3	2.07	0.54
1:A:46:LEU:HD13	2:A:601:FAD:HM81	1.89	0.53
1:E:454:GLU:N	1:E:454:GLU:OE2	2.20	0.53
1:H:500:GLY:O	1:H:504:PHE:CD2	2.61	0.53
1:E:291:PHE:CG	1:E:292:TYR:N	2.76	0.53
1:B:159:MET:CE	3:B:602:GDU:N3	2.71	0.53
1:F:122:ILE:O	1:F:126:ILE:HG13	2.08	0.53
1:D:178:TRP:CB	1:D:454:GLU:HG3	2.35	0.53
1:H:471:ASN:HA	1:H:476:ALA:H	1.73	0.53
1:B:325:PHE:HA	1:B:374:VAL:HG22	1.89	0.53
1:H:158:PHE:CD1	1:H:158:PHE:C	2.82	0.53
1:G:158:PHE:CG	1:G:159:MET:SD	3.01	0.53
1:H:95:VAL:HG22	1:H:317:TYR:HD2	1.72	0.53
1:D:134:VAL:CG1	1:D:134:VAL:O	2.56	0.53
1:H:348:THR:HB	1:H:357:PRO:HB3	1.90	0.53
1:D:242:VAL:HA	1:D:254:LEU:CD2	2.38	0.53
1:G:500:GLY:O	1:G:504:PHE:CD2	2.62	0.53
1:A:455:VAL:CG1	1:A:464:LEU:HD11	2.38	0.53
1:D:398:THR:O	1:D:398:THR:HG22	2.08	0.53
1:H:283:LEU:O	1:H:287:THR:HG23	2.08	0.53
1:G:367:TYR:CE1	1:G:408:VAL:HG11	2.43	0.53
1:A:269:MET:HG2	1:A:274:LEU:HD22	1.91	0.53
1:D:6:ILE:O	1:D:260:ILE:HA	2.09	0.53
1:F:162:TYR:O	1:F:166:VAL:HG12	2.08	0.53
1:H:417:HIS:HB3	1:H:448:PHE:CZ	2.42	0.53
1:G:306:ARG:HD2	1:G:311:GLY:O	2.09	0.53
1:B:395:LEU:HA	1:B:400:MET:HG3	1.91	0.53
1:H:28:GLN:NE2	1:H:502:GLN:OE1	2.41	0.53
1:C:417:HIS:HB3	1:C:448:PHE:CZ	2.44	0.53
1:A:155:ALA:O	1:A:160:ARG:HG3	2.08	0.53
1:H:479:LEU:HA	1:H:483:TYR:HD2	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLN:HG3	1:D:422:PRO:O	2.09	0.53
1:H:58:TYR:CE1	1:H:369:SER:OG	2.61	0.53
1:B:91:ARG:HD3	1:B:207:ASN:CB	2.36	0.53
1:C:350:GLN:NE2	1:C:354:GLY:HA2	2.21	0.53
1:H:342:ALA:O	1:H:365:GLY:O	2.27	0.53
1:D:468:ALA:O	1:D:472:ILE:HG13	2.09	0.53
1:B:16:GLY:HA3	2:B:601:FAD:PA	2.48	0.53
1:G:17:PRO:N	2:G:601:FAD:O1P	2.42	0.53
1:G:63:HIS:HB2	1:G:218:THR:HG21	1.91	0.53
1:A:93:SER:HB2	1:A:104:TYR:HB3	1.90	0.53
1:A:419:TYR:HE1	2:A:601:FAD:HM73	1.74	0.53
1:D:113:LEU:O	1:D:118:GLN:NE2	2.31	0.53
1:E:353:ASP:HB3	1:E:403:PRO:HB3	1.89	0.53
1:C:455:VAL:CG1	1:C:455:VAL:O	2.55	0.53
1:G:250:LYS:HD2	1:G:262:TYR:CE1	2.44	0.53
1:E:137:THR:C	1:E:148:ARG:HH12	2.11	0.53
1:C:63:HIS:CD2	2:C:601:FAD:C5X	2.92	0.53
1:A:108:ASN:HD22	1:A:201:ALA:HB3	1.73	0.53
1:F:165:LYS:HZ3	1:F:318:PHE:HB3	1.74	0.53
1:E:219:GLY:O	1:E:223:ILE:HG12	2.09	0.53
1:G:116:GLU:OE2	1:G:117:GLU:HG2	2.08	0.53
1:F:192:THR:O	1:F:196:ILE:HG13	2.08	0.53
1:D:107:GLN:CD	1:D:107:GLN:H	2.10	0.53
1:G:351:LEU:HD12	1:G:404:THR:HA	1.90	0.53
1:A:163:ASN:HA	1:A:166:VAL:CG1	2.38	0.53
1:A:43:PRO:HG2	1:A:223:ILE:HD13	1.89	0.53
1:C:344:LYS:HD2	1:C:345:LYS:N	2.24	0.53
1:C:39:SER:HB3	1:C:241:LYS:HG2	1.90	0.53
1:D:242:VAL:HA	1:D:254:LEU:HD22	1.90	0.53
1:A:58:TYR:HA	1:A:331:PHE:CE2	2.42	0.53
1:H:28:GLN:HG3	1:H:497:LEU:HD12	1.91	0.53
1:D:196:ILE:HD12	1:F:119:VAL:HG22	1.91	0.53
1:E:387:ILE:HG23	1:E:388:LEU:H	1.71	0.53
1:F:142:PHE:CB	1:F:174:MET:HB2	2.39	0.53
1:E:326:TYR:N	1:E:374:VAL:HG13	2.23	0.53
1:C:182:ARG:HD2	3:C:602:GDU:PA	2.49	0.53
1:G:149:MET:SD	1:G:184:ALA:CA	2.94	0.53
1:F:323:CYS:HB2	1:F:324:PRO:HD2	1.90	0.53
1:G:337:TYR:CD1	1:G:337:TYR:N	2.76	0.53
1:H:323:CYS:HB2	1:H:325:PHE:CZ	2.44	0.53
1:C:242:VAL:H	2:C:601:FAD:H62A	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:66:PHE:CB	1:E:206:PRO:O	2.57	0.53
1:A:242:VAL:HA	1:A:254:LEU:CD2	2.39	0.53
1:C:383:ASN:O	1:C:387:ILE:HB	2.08	0.53
1:F:70:LYS:HB3	1:F:496:ARG:NH1	2.25	0.52
1:B:143:ASP:O	1:B:147:VAL:HG23	2.08	0.52
1:H:338:ASN:HB2	1:H:339:GLN:HE22	1.73	0.52
1:D:38:ASP:HA	2:D:601:FAD:H2A	1.91	0.52
1:H:411:TYR:HD1	1:H:411:TYR:C	2.11	0.52
1:H:160:ARG:HB2	1:H:161:PRO:HD3	1.91	0.52
1:G:322:ASN:ND2	1:G:397:ASN:HB3	2.23	0.52
1:G:389:ALA:O	1:G:392:ILE:HB	2.09	0.52
1:H:28:GLN:NE2	1:H:497:LEU:O	2.37	0.52
1:H:349:MET:SD	1:H:409:SER:HA	2.49	0.52
1:B:38:ASP:OD2	1:B:40:ASN:HB2	2.08	0.52
1:H:492:ASN:ND2	1:H:492:ASN:N	2.56	0.52
1:E:38:ASP:OD2	1:E:40:ASN:N	2.42	0.52
1:E:159:MET:CE	3:E:602:GDU:C2	2.88	0.52
1:G:249:ASN:N	1:G:249:ASN:OD1	2.42	0.52
1:A:455:VAL:O	1:A:455:VAL:CG1	2.56	0.52
1:G:64:VAL:HG22	1:G:210:PHE:CD1	2.44	0.52
1:B:87:TYR:HB3	1:B:89:HIS:CE1	2.44	0.52
1:F:129:ALA:O	1:F:132:ALA:HB3	2.08	0.52
1:G:18:THR:HG21	1:G:268:THR:CG2	2.32	0.52
1:G:194:ASN:ND2	1:G:199:LYS:O	2.42	0.52
1:G:189:LYS:O	1:G:193:THR:OG1	2.23	0.52
1:G:25:ARG:HD3	1:G:470:ASP:OD1	2.09	0.52
1:E:12:VAL:O	1:E:36:ILE:HA	2.09	0.52
1:D:11:LEU:O	1:D:265:LEU:HD12	2.09	0.52
1:E:19:GLY:H	1:E:268:THR:HG21	1.72	0.52
1:E:167:TRP:CD2	1:E:174:MET:HE1	2.44	0.52
1:G:160:ARG:HB2	1:G:161:PRO:HD3	1.92	0.52
1:H:70:LYS:HB2	1:H:493:THR:HA	1.90	0.52
1:A:152:THR:HG22	1:A:156:ASP:OD2	2.09	0.52
1:C:110:ILE:CA	1:C:113:LEU:HD12	2.35	0.52
1:A:466:VAL:HG12	1:A:495:ARG:NH1	2.25	0.52
1:H:163:ASN:O	1:H:167:TRP:HB2	2.09	0.52
1:C:242:VAL:HA	1:C:254:LEU:HD22	1.91	0.52
1:E:204:TRP:CE3	1:E:205:GLY:HA2	2.44	0.52
1:H:283:LEU:HD22	1:H:433:ILE:HG23	1.91	0.52
1:D:163:ASN:HA	1:D:166:VAL:CG1	2.39	0.52
1:F:349:MET:N	1:F:407:ILE:O	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:HIS:O	1:D:492:ASN:ND2	2.40	0.52
1:F:325:PHE:HA	1:F:374:VAL:CG1	2.40	0.52
1:E:22:ALA:O	1:E:26:LEU:HB2	2.08	0.52
1:A:245:VAL:HG22	1:A:252:VAL:HG23	1.90	0.52
1:H:455:VAL:HG13	1:H:484:PRO:HB3	1.91	0.52
1:D:16:GLY:CA	2:D:601:FAD:H52A	2.38	0.52
1:H:389:ALA:O	1:H:392:ILE:HB	2.10	0.52
1:G:253:THR:HA	1:G:259:THR:HG22	1.92	0.52
1:B:103:PRO:HB2	1:B:109:ASN:ND2	2.25	0.52
1:F:313:LYS:O	1:F:333:ASN:ND2	2.42	0.52
1:A:199:LYS:HD2	1:A:200:THR:O	2.09	0.52
1:C:114:PRO:O	1:C:118:GLN:HG3	2.09	0.52
1:E:69:TYR:HB2	1:E:72:PHE:HB3	1.91	0.52
1:A:416:ASP:HB2	1:F:281:GLN:HE21	1.75	0.52
1:E:427:GLU:O	1:E:431:THR:HG23	2.09	0.52
1:G:89:HIS:NE2	1:G:334:TYR:HA	2.25	0.52
1:C:175:GLN:HG3	1:C:422:PRO:O	2.10	0.52
1:B:125:MET:CE	1:B:186:PRO:HB2	2.40	0.52
1:E:142:PHE:O	1:E:146:ILE:HG13	2.10	0.52
1:E:167:TRP:HE3	1:E:421:THR:HG22	1.74	0.52
1:E:335:SER:HB3	1:E:338:ASN:OD1	2.09	0.52
1:G:79:ALA:HB2	1:G:225:VAL:CG2	2.38	0.52
1:F:303:ARG:HH21	1:F:363:LYS:C	2.13	0.52
1:G:8:VAL:O	1:G:262:TYR:HA	2.10	0.52
1:A:395:LEU:HD22	1:A:400:MET:HE2	1.92	0.52
1:C:307:PRO:HD2	1:C:310:ILE:HD12	1.91	0.52
1:A:28:GLN:NE2	1:A:502:GLN:OE1	2.42	0.52
1:F:82:LYS:HB2	1:F:85:ASP:OD2	2.09	0.52
1:B:134:VAL:O	1:B:134:VAL:CG1	2.57	0.52
1:F:19:GLY:CA	1:F:268:THR:HG21	2.40	0.52
1:A:183:VAL:HG22	3:A:602:GDU:H1D	1.92	0.52
1:B:504:PHE:CZ	1:F:264:LYS:HG2	2.43	0.52
1:E:298:ILE:CD1	1:E:388:LEU:HD13	2.40	0.52
1:F:306:ARG:NH1	1:F:333:ASN:OD1	2.42	0.52
1:E:24:LYS:HE3	1:E:229:LEU:HD21	1.92	0.52
1:F:158:PHE:O	1:F:161:PRO:HG2	2.10	0.52
1:H:270:ALA:HB1	1:H:272:ASP:OD1	2.09	0.52
1:D:455:VAL:HG21	1:D:480:THR:O	2.10	0.52
1:F:10:VAL:HG22	1:F:264:LYS:HG3	1.92	0.52
1:D:336:PRO:HG2	1:D:337:TYR:CD1	2.45	0.52
1:B:346:LEU:HD23	1:B:347:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:PHE:HZ	1:G:334:TYR:CE1	2.28	0.52
1:A:344:LYS:HD2	1:A:345:LYS:N	2.25	0.52
1:H:254:LEU:HB2	1:H:258:THR:HB	1.91	0.52
1:F:453:TYR:O	1:F:453:TYR:CD2	2.62	0.52
1:E:18:THR:HA	1:E:461:SER:O	2.09	0.51
1:D:271:VAL:HA	1:D:274:LEU:HB2	1.92	0.51
1:G:244:LYS:HB3	1:G:253:THR:HB	1.91	0.51
1:B:199:LYS:HD2	1:B:200:THR:O	2.10	0.51
1:F:110:ILE:HG23	1:F:195:VAL:HG22	1.93	0.51
1:E:504:PHE:N	1:E:504:PHE:CD1	2.78	0.51
1:G:453:TYR:CD2	1:G:453:TYR:O	2.63	0.51
1:D:40:ASN:O	1:D:236:PHE:HB3	2.09	0.51
1:G:455:VAL:HA	1:G:460:HIS:ND1	2.24	0.51
1:G:375:SER:OG	1:G:380:LYS:HE3	2.11	0.51
1:G:283:LEU:O	1:G:287:THR:HG23	2.10	0.51
1:C:155:ALA:O	1:C:160:ARG:HG3	2.10	0.51
1:F:38:ASP:OD1	2:F:601:FAD:H1B	2.11	0.51
1:F:21:GLY:HA2	1:F:462:PHE:CE1	2.45	0.51
1:G:38:ASP:OD2	1:G:39:SER:N	2.43	0.51
1:H:272:ASP:OD1	1:H:272:ASP:N	2.40	0.51
1:G:376:GLU:CG	1:G:382:VAL:HG13	2.37	0.51
1:E:150:MET:O	1:E:154:ILE:HG13	2.10	0.51
1:D:325:PHE:CZ	1:D:395:LEU:HD23	2.45	0.51
1:E:269:MET:CE	1:E:273:PHE:HB3	2.39	0.51
1:B:346:LEU:HD23	1:B:347:PRO:CD	2.40	0.51
1:B:242:VAL:HA	1:B:254:LEU:HD22	1.93	0.51
1:D:183:VAL:HG22	3:D:602:GDU:H1D	1.93	0.51
1:B:232:GLU:CD	1:B:232:GLU:H	2.13	0.51
1:E:133:ARG:CG	1:E:133:ARG:NH1	2.71	0.51
1:H:143:ASP:O	1:H:147:VAL:HG23	2.10	0.51
1:B:395:LEU:HD22	1:B:400:MET:CE	2.40	0.51
1:C:398:THR:HB	1:C:400:MET:HG3	1.93	0.51
1:H:250:LYS:O	1:H:261:GLY:HA2	2.10	0.51
1:A:32:PRO:HG3	1:E:504:PHE:HD2	1.75	0.51
1:E:291:PHE:CE1	1:E:292:TYR:O	2.64	0.51
1:F:458:GLN:HG3	2:F:601:FAD:H1'2	1.91	0.51
1:E:320:GLU:HB2	1:E:322:ASN:OD1	2.11	0.51
1:C:242:VAL:HA	1:C:254:LEU:CD2	2.41	0.51
1:F:272:ASP:N	1:F:272:ASP:OD1	2.43	0.51
1:F:167:TRP:HE3	1:F:421:THR:HG22	1.75	0.51
1:E:281:GLN:OE1	1:E:284:VAL:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:GLY:HA3	2:D:601:FAD:O1P	2.11	0.51
1:A:192:THR:OG1	1:A:193:THR:N	2.43	0.51
1:C:306:ARG:CZ	1:C:311:GLY:HA2	2.40	0.51
1:D:212:PHE:CG	1:D:213:PRO:HD2	2.46	0.51
1:F:391:CYS:O	1:F:395:LEU:HG	2.11	0.51
1:G:9:ASP:OD1	1:G:33:SER:N	2.43	0.51
1:D:272:ASP:N	1:D:272:ASP:OD1	2.44	0.51
1:G:18:THR:HB	2:G:601:FAD:O2P	2.11	0.51
1:D:494:GLU:HG2	1:H:477:VAL:HA	1.93	0.51
1:A:69:TYR:CD2	1:A:463:MET:HG3	2.46	0.51
1:F:204:TRP:CE3	1:F:205:GLY:N	2.79	0.51
1:A:189:LYS:HE2	1:G:123:ASP:HA	1.92	0.51
1:H:244:LYS:HB3	1:H:253:THR:HB	1.92	0.51
1:G:95:VAL:HG22	1:G:317:TYR:HD2	1.75	0.51
1:F:15:ALA:H	2:F:601:FAD:H4B	1.75	0.51
1:G:447:ARG:HG2	1:G:448:PHE:CE2	2.45	0.51
2:G:601:FAD:O1A	2:G:601:FAD:O1P	2.29	0.51
1:D:63:HIS:HB3	1:D:458:GLN:NE2	2.26	0.51
1:F:149:MET:O	1:F:149:MET:HG2	2.11	0.51
1:D:192:THR:OG1	1:D:193:THR:N	2.44	0.51
1:G:383:ASN:ND2	1:G:386:THR:HG23	2.25	0.51
1:G:15:ALA:HB2	1:G:38:ASP:HB2	1.91	0.50
1:D:91:ARG:O	1:D:92:ILE:HD13	2.11	0.50
1:F:230:PRO:CG	1:F:233:LYS:HD2	2.37	0.50
1:C:325:PHE:CZ	1:C:395:LEU:HD23	2.45	0.50
1:H:438:GLN:HA	1:H:442:ILE:O	2.10	0.50
1:B:455:VAL:O	1:B:455:VAL:CG1	2.59	0.50
1:B:303:ARG:NH2	1:B:363:LYS:O	2.43	0.50
1:H:253:THR:HA	1:H:259:THR:HG22	1.93	0.50
1:H:175:GLN:O	1:H:178:TRP:NE1	2.44	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH1	2.26	0.50
1:G:39:SER:HB3	1:G:241:LYS:CB	2.41	0.50
1:G:204:TRP:HE3	1:G:204:TRP:HA	1.75	0.50
1:E:309:ARG:H	1:E:309:ARG:HD3	1.76	0.50
1:G:158:PHE:HE1	1:G:162:TYR:CG	2.28	0.50
1:B:304:GLY:O	1:B:368:TRP:HD1	1.95	0.50
1:C:212:PHE:CG	1:C:213:PRO:HD2	2.46	0.50
1:G:16:GLY:O	1:G:20:LEU:HG	2.10	0.50
1:D:155:ALA:O	1:D:160:ARG:HG3	2.12	0.50
1:D:432:GLN:O	1:D:436:LYS:HB2	2.11	0.50
1:F:18:THR:HA	1:F:461:SER:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PRO:O	1:E:374:VAL:HG11	2.10	0.50
1:C:182:ARG:NH1	3:C:602:GDU:O2'	2.43	0.50
1:B:192:THR:O	1:B:196:ILE:HG13	2.12	0.50
1:F:454:GLU:OE2	1:F:454:GLU:N	2.26	0.50
1:D:108:ASN:HD22	1:D:201:ALA:HB3	1.75	0.50
1:E:204:TRP:CE3	1:E:205:GLY:N	2.79	0.50
1:A:307:PRO:HD2	1:A:310:ILE:HD12	1.93	0.50
1:C:6:ILE:O	1:C:260:ILE:HA	2.10	0.50
1:B:244:LYS:HG2	1:B:245:VAL:N	2.26	0.50
1:D:306:ARG:CZ	1:D:311:GLY:HA2	2.41	0.50
1:F:82:LYS:HB2	1:F:85:ASP:CG	2.30	0.50
1:B:95:VAL:HG23	1:B:102:VAL:O	2.10	0.50
1:D:87:TYR:HB3	1:D:89:HIS:CE1	2.46	0.50
1:D:150:MET:HG2	1:D:154:ILE:HG21	1.93	0.50
1:B:64:VAL:HG13	1:B:210:PHE:CD1	2.46	0.50
1:F:38:ASP:OD2	1:F:40:ASN:N	2.41	0.50
1:H:38:ASP:OD1	2:H:601:FAD:O3B	2.23	0.50
1:H:309:ARG:HG2	1:H:310:ILE:CD1	2.42	0.50
1:C:139:PRO:HB2	1:C:176:CYS:SG	2.51	0.50
1:B:455:VAL:HG13	1:B:455:VAL:O	2.11	0.50
1:F:411:TYR:OH	1:F:413:ARG:HB3	2.11	0.50
1:F:397:ASN:C	1:F:399:GLU:H	2.14	0.50
1:D:447:ARG:O	1:D:451:TRP:HA	2.11	0.50
1:E:244:LYS:HG2	1:E:245:VAL:N	2.26	0.50
1:F:443:TRP:CE3	1:F:443:TRP:N	2.79	0.50
1:B:183:VAL:HG13	3:B:602:GDU:O2	2.09	0.50
1:H:464:LEU:HD21	1:H:481:LEU:CA	2.41	0.50
1:G:299:GLY:HA2	1:G:370:ILE:O	2.11	0.50
1:B:346:LEU:HD13	1:B:408:VAL:HG13	1.93	0.50
1:D:504:PHE:HA	1:D:507:SER:HB3	1.92	0.50
1:H:425:GLU:CD	1:H:425:GLU:N	2.64	0.50
2:F:601:FAD:O2'	2:F:601:FAD:H9	2.11	0.50
1:G:150:MET:O	1:G:154:ILE:HD13	2.11	0.50
1:E:270:ALA:HB3	1:E:273:PHE:CD2	2.47	0.50
1:H:335:SER:HB3	1:H:338:ASN:OD1	2.11	0.50
1:G:181:GLU:HA	1:G:181:GLU:OE1	2.12	0.50
1:C:103:PRO:CG	1:C:109:ASN:ND2	2.72	0.50
1:F:76:LEU:HD12	1:F:211:ARG:NH2	2.27	0.50
1:H:453:TYR:O	1:H:453:TYR:CD2	2.64	0.50
1:C:199:LYS:HD2	1:C:200:THR:O	2.12	0.50
1:F:136:ASN:OD1	1:F:137:THR:HG23	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:VAL:HA	1:F:326:TYR:CD2	2.47	0.50
1:G:479:LEU:HA	1:G:483:TYR:HD2	1.76	0.50
1:G:455:VAL:HG21	1:G:480:THR:O	2.12	0.50
1:B:178:TRP:CB	1:B:454:GLU:HG3	2.35	0.50
1:G:332:SER:HA	1:G:339:GLN:HE22	1.76	0.50
1:E:359:SER:HB3	1:E:363:LYS:HE2	1.93	0.50
1:H:181:GLU:N	1:H:485:ASP:OD1	2.44	0.50
1:E:122:ILE:HG22	1:E:123:ASP:N	2.27	0.50
1:B:212:PHE:CG	1:B:213:PRO:HD2	2.47	0.50
1:C:152:THR:HG22	1:C:156:ASP:OD2	2.11	0.50
1:E:224:ALA:O	1:E:228:THR:HG23	2.12	0.50
1:E:467:GLU:HG2	1:E:495:ARG:NH2	2.26	0.50
1:B:16:GLY:HA3	2:B:601:FAD:O5B	2.11	0.50
1:F:71:TYR:HB2	1:F:495:ARG:O	2.11	0.50
1:F:122:ILE:CG2	1:F:123:ASP:N	2.75	0.50
1:H:61:GLY:HA3	2:H:601:FAD:C6	2.41	0.50
1:H:351:LEU:HD12	1:H:404:THR:HA	1.93	0.50
1:D:455:VAL:CG1	1:D:455:VAL:O	2.59	0.50
1:C:192:THR:O	1:C:196:ILE:HG13	2.11	0.50
1:C:69:TYR:CD2	1:C:463:MET:HG3	2.47	0.50
1:C:143:ASP:O	1:C:147:VAL:HG23	2.11	0.50
1:E:413:ARG:HG2	1:E:414:ARG:N	2.26	0.50
1:G:128:ALA:HB2	1:G:151:GLY:HA2	1.93	0.50
1:D:483:TYR:N	1:D:484:PRO:HD3	2.27	0.50
1:H:178:TRP:HD1	1:H:178:TRP:H	1.60	0.50
1:D:160:ARG:N	1:D:161:PRO:HD2	2.26	0.50
1:B:175:GLN:HG3	1:B:422:PRO:O	2.12	0.50
1:G:109:ASN:HD21	1:G:201:ALA:C	2.14	0.50
1:H:167:TRP:O	1:H:169:VAL:HG12	2.12	0.50
1:C:108:ASN:ND2	1:C:201:ALA:HB3	2.27	0.50
1:B:296:HIS:NE2	1:B:382:VAL:HG21	2.27	0.50
1:F:110:ILE:CG2	1:F:195:VAL:HG22	2.42	0.50
1:D:244:LYS:HG2	1:D:245:VAL:N	2.27	0.50
1:H:345:LYS:HE3	1:H:364:GLU:OE1	2.12	0.50
1:F:326:TYR:N	1:F:374:VAL:HG13	2.26	0.49
1:H:455:VAL:HA	1:H:460:HIS:ND1	2.27	0.49
1:G:351:LEU:HD13	1:G:404:THR:O	2.11	0.49
1:G:251:THR:HA	1:G:260:ILE:O	2.12	0.49
1:C:103:PRO:HB2	1:C:109:ASN:HD21	1.73	0.49
1:G:262:TYR:CE1	1:G:265:LEU:HB2	2.47	0.49
1:F:114:PRO:O	1:F:118:GLN:HG3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:GLY:HA3	2:F:601:FAD:O5B	2.11	0.49
1:G:270:ALA:HB1	1:G:272:ASP:OD1	2.12	0.49
1:H:292:TYR:CE1	1:H:417:HIS:ND1	2.79	0.49
1:H:61:GLY:HA2	1:H:373:GLU:OE1	2.12	0.49
1:D:455:VAL:O	1:D:455:VAL:HG13	2.11	0.49
1:H:411:TYR:CD1	1:H:412:HIS:N	2.70	0.49
1:B:269:MET:HG2	1:B:274:LEU:HD22	1.94	0.49
1:C:57:LEU:N	1:C:57:LEU:CD1	2.75	0.49
1:B:499:ASP:O	1:B:503:VAL:HG23	2.11	0.49
1:F:396:VAL:HA	1:F:401:LEU:HB2	1.94	0.49
1:D:152:THR:HG22	1:D:156:ASP:OD2	2.11	0.49
1:G:292:TYR:CZ	1:G:417:HIS:CE1	3.00	0.49
1:D:58:TYR:HA	1:D:331:PHE:CE2	2.46	0.49
1:F:91:ARG:CZ	1:F:93:SER:HB2	2.42	0.49
1:G:71:TYR:CE2	1:G:497:LEU:HA	2.47	0.49
1:G:401:LEU:HA	1:G:405:ASP:OD2	2.13	0.49
1:G:402:LYS:H	1:G:402:LYS:HD3	1.78	0.49
1:G:64:VAL:HG22	1:G:210:PHE:CE1	2.47	0.49
1:B:72:PHE:CE2	1:B:76:LEU:HD11	2.48	0.49
1:G:63:HIS:H	1:G:63:HIS:CD2	2.30	0.49
1:G:104:TYR:CD2	1:G:105:PRO:HA	2.46	0.49
1:A:241:LYS:HE3	2:A:601:FAD:N6A	2.28	0.49
1:E:303:ARG:NH1	1:E:348:THR:OG1	2.45	0.49
1:G:125:MET:HG2	1:G:188:LEU:HG	1.94	0.49
1:G:28:GLN:NE2	1:G:502:GLN:OE1	2.45	0.49
1:H:11:LEU:HB3	1:H:265:LEU:HD12	1.93	0.49
1:F:269:MET:CE	1:F:273:PHE:HB3	2.42	0.49
1:F:15:ALA:N	2:F:601:FAD:H4B	2.27	0.49
1:A:244:LYS:HG2	1:A:245:VAL:N	2.27	0.49
1:B:196:ILE:HG21	1:H:119:VAL:HG22	1.95	0.49
1:G:393:GLN:NE2	1:G:397:ASN:OD1	2.45	0.49
1:G:71:TYR:HB2	1:G:495:ARG:O	2.11	0.49
1:A:325:PHE:CZ	1:A:395:LEU:HD23	2.48	0.49
1:E:411:TYR:OH	1:E:413:ARG:HB3	2.13	0.49
1:F:460:HIS:O	1:F:463:MET:HB2	2.11	0.49
1:E:397:ASN:C	1:E:399:GLU:H	2.16	0.49
1:D:178:TRP:HB2	1:D:454:GLU:CG	2.38	0.49
1:G:54:GLU:N	1:G:54:GLU:OE2	2.45	0.49
1:F:508:LYS:HG3	1:F:509:ALA:N	2.27	0.49
1:D:95:VAL:HG23	1:D:102:VAL:O	2.13	0.49
1:D:352:ALA:HB3	1:D:403:PRO:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:LEU:HB2	1:F:425:GLU:OE1	2.12	0.49
1:A:346:LEU:HD23	1:A:347:PRO:HD2	1.93	0.49
1:H:460:HIS:CE1	1:H:488:ASN:OD1	2.66	0.49
1:H:48:SER:O	1:H:60:VAL:HG23	2.13	0.49
1:F:56:PHE:CE2	1:F:409:SER:HB3	2.46	0.49
1:H:28:GLN:HE21	1:H:497:LEU:C	2.15	0.49
1:B:307:PRO:HB2	1:B:309:ARG:HG2	1.95	0.49
1:E:173:LYS:HA	1:E:424:LEU:HD11	1.95	0.49
1:D:388:LEU:O	1:D:392:ILE:HG13	2.13	0.49
1:F:26:LEU:HG	1:F:469:VAL:HG13	1.94	0.49
1:C:178:TRP:CB	1:C:454:GLU:CG	2.90	0.49
1:G:58:TYR:CE1	1:G:369:SER:OG	2.63	0.49
1:H:104:TYR:CD2	1:H:105:PRO:HA	2.46	0.49
1:C:103:PRO:HG2	1:C:109:ASN:CG	2.33	0.49
1:C:142:PHE:HE2	1:C:163:ASN:ND2	2.10	0.49
1:B:504:PHE:CZ	1:F:264:LYS:CG	2.96	0.49
1:H:11:LEU:HB3	1:H:265:LEU:CD1	2.43	0.49
1:B:414:ARG:HH12	1:B:416:ASP:HA	1.78	0.49
1:D:330:ILE:HB	1:D:333:ASN:OD1	2.13	0.49
1:E:18:THR:O	1:E:465:GLY:HA3	2.13	0.49
1:A:346:LEU:HD23	1:A:347:PRO:CD	2.43	0.49
1:G:418:GLY:O	1:G:419:TYR:HD1	1.96	0.49
1:G:467:GLU:CD	1:G:480:THR:H	2.12	0.49
1:E:9:ASP:CA	1:E:263:LYS:HD3	2.37	0.49
1:H:332:SER:OG	1:H:368:TRP:HB2	2.13	0.49
1:F:179:LEU:HD23	1:F:179:LEU:H	1.78	0.49
1:A:178:TRP:CH2	1:A:179:LEU:HD23	2.48	0.49
1:G:126:ILE:HA	1:G:188:LEU:HD11	1.95	0.49
1:D:69:TYR:CD2	1:D:463:MET:HG3	2.48	0.49
1:G:11:LEU:HD21	1:G:252:VAL:CG1	2.43	0.49
1:H:322:ASN:ND2	1:H:397:ASN:HB3	2.26	0.49
1:B:57:LEU:HD13	1:B:338:ASN:O	2.13	0.49
1:D:351:LEU:HB2	1:D:355:SER:OG	2.13	0.49
1:F:19:GLY:H	1:F:268:THR:HG21	1.73	0.49
1:E:17:PRO:O	1:E:462:PHE:CD1	2.66	0.49
1:A:346:LEU:HD13	1:A:408:VAL:HG13	1.94	0.49
1:H:484:PRO:HA	1:H:487:VAL:CG2	2.43	0.49
1:H:38:ASP:OD2	1:H:39:SER:N	2.46	0.49
1:D:175:GLN:NE2	1:D:178:TRP:HD1	2.10	0.49
1:G:142:PHE:HA	1:G:176:CYS:HB3	1.94	0.49
1:F:187:ASN:O	1:F:191:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:THR:HA	1:D:487:VAL:HG11	1.95	0.49
1:C:455:VAL:O	1:C:460:HIS:CB	2.61	0.49
1:H:203:ASN:ND2	1:H:204:TRP:H	2.08	0.49
1:G:290:LEU:HD21	1:G:430:LEU:HD23	1.94	0.49
1:H:290:LEU:HD21	1:H:430:LEU:HD23	1.95	0.49
1:G:2:THR:OG1	1:G:3:HIS:N	2.46	0.49
1:F:163:ASN:ND2	3:F:602:GDU:O2D	2.42	0.48
1:B:17:PRO:HG2	2:B:601:FAD:O4'	2.13	0.48
1:A:178:TRP:CB	1:A:454:GLU:HG3	2.38	0.48
1:G:332:SER:OG	1:G:368:TRP:HB2	2.13	0.48
1:F:108:ASN:C	1:F:194:ASN:HD22	2.17	0.48
1:A:463:MET:O	1:A:467:GLU:HG3	2.13	0.48
1:G:71:TYR:CD2	1:G:496:ARG:C	2.86	0.48
1:G:28:GLN:HG3	1:G:497:LEU:HD12	1.95	0.48
1:H:100:GLN:HA	1:H:100:GLN:OE1	2.13	0.48
1:C:346:LEU:HD13	1:C:408:VAL:HG13	1.95	0.48
1:A:272:ASP:N	1:A:272:ASP:OD1	2.45	0.48
1:G:464:LEU:HD21	1:G:481:LEU:CA	2.44	0.48
1:C:178:TRP:CB	1:C:454:GLU:HG3	2.36	0.48
1:F:303:ARG:HH21	1:F:363:LYS:CA	2.26	0.48
1:H:28:GLN:CG	1:H:497:LEU:O	2.62	0.48
1:A:395:LEU:HA	1:A:400:MET:HG3	1.94	0.48
1:F:350:GLN:NE2	1:F:407:ILE:HD12	2.28	0.48
1:D:125:MET:CE	1:D:186:PRO:HB2	2.43	0.48
1:B:272:ASP:N	1:B:272:ASP:OD1	2.47	0.48
1:G:197:LEU:HB2	1:G:199:LYS:HB3	1.95	0.48
1:H:492:ASN:HD22	1:H:492:ASN:N	2.10	0.48
1:C:116:GLU:O	1:C:119:VAL:HB	2.13	0.48
1:E:434:LEU:N	1:E:435:PRO:HD2	2.28	0.48
1:C:458:GLN:HG3	2:C:601:FAD:N1	2.28	0.48
1:F:69:TYR:CD1	1:F:463:MET:HG3	2.48	0.48
1:B:250:LYS:HD3	1:B:262:TYR:O	2.13	0.48
1:H:86:TRP:HA	1:H:86:TRP:CE3	2.49	0.48
1:D:477:VAL:HA	1:H:494:GLU:HG2	1.93	0.48
1:E:443:TRP:N	1:E:443:TRP:CE3	2.81	0.48
2:B:601:FAD:H6	3:B:602:GDU:O3'	2.12	0.48
1:G:242:VAL:HG13	1:G:252:VAL:HG22	1.94	0.48
1:D:395:LEU:HD22	1:D:400:MET:HE2	1.95	0.48
1:C:232:GLU:N	1:C:232:GLU:OE2	2.45	0.48
1:C:87:TYR:HB3	1:C:89:HIS:CE1	2.48	0.48
1:C:5:ASP:OD2	1:C:258:THR:HA	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:PHE:CE1	1:A:339:GLN:HB3	2.49	0.48
1:E:322:ASN:HD21	1:E:398:THR:HG22	1.77	0.48
1:B:196:ILE:HD12	1:H:119:VAL:HG22	1.96	0.48
1:E:331:PHE:CE2	1:E:338:ASN:ND2	2.82	0.48
1:G:234:THR:HB	1:G:236:PHE:CE2	2.48	0.48
1:G:28:GLN:HG2	1:G:497:LEU:O	2.13	0.48
1:A:475:GLY:O	1:E:494:GLU:HB2	2.14	0.48
1:B:336:PRO:HG2	1:B:337:TYR:CD1	2.49	0.48
1:E:63:HIS:CE1	2:E:601:FAD:C5X	2.97	0.48
1:G:141:THR:OG1	1:G:144:GLU:HB2	2.13	0.48
1:D:47:ALA:HB1	1:D:222:TRP:NE1	2.27	0.48
1:H:250:LYS:HD2	1:H:262:TYR:CE1	2.48	0.48
1:H:242:VAL:HG13	1:H:252:VAL:HG22	1.96	0.48
1:H:425:GLU:CD	1:H:425:GLU:H	2.17	0.48
1:C:8:VAL:HG11	1:C:35:MET:HG2	1.96	0.48
1:E:70:LYS:HD2	1:E:70:LYS:HA	1.55	0.48
1:F:324:PRO:O	1:F:374:VAL:HG11	2.13	0.48
1:G:270:ALA:HA	1:G:448:PHE:C	2.34	0.48
1:D:56:PHE:CE1	1:D:339:GLN:HB3	2.49	0.48
1:E:269:MET:HE1	2:E:601:FAD:H61A	1.79	0.48
1:A:39:SER:HB3	1:A:241:LYS:HG2	1.95	0.48
1:E:189:LYS:O	1:E:192:THR:OG1	2.20	0.48
1:F:387:ILE:HG23	1:F:388:LEU:N	2.28	0.48
1:C:224:ALA:O	1:C:228:THR:HG23	2.14	0.48
1:B:437:LEU:CD1	1:B:444:SER:HB2	2.44	0.48
1:G:17:PRO:HG2	2:G:601:FAD:H4'	1.96	0.48
1:H:467:GLU:CD	1:H:480:THR:H	2.10	0.48
1:G:58:TYR:CZ	1:G:299:GLY:HA3	2.48	0.48
1:H:158:PHE:C	1:H:158:PHE:HD1	2.15	0.48
1:B:47:ALA:CB	1:B:222:TRP:NE1	2.76	0.48
1:E:376:GLU:HG2	1:E:377:SER:N	2.28	0.48
1:F:167:TRP:O	1:F:169:VAL:HG13	2.13	0.48
1:A:39:SER:CB	1:A:241:LYS:HG2	2.43	0.48
1:G:394:GLY:HA2	1:G:397:ASN:HB2	1.95	0.48
1:C:466:VAL:HG12	1:C:495:ARG:NH1	2.29	0.48
1:F:69:TYR:CE2	1:F:463:MET:HG3	2.48	0.48
1:A:32:PRO:HB3	1:E:504:PHE:HD2	1.78	0.48
1:A:87:TYR:HB3	1:A:89:HIS:HE1	1.79	0.48
1:F:235:ARG:HG2	1:F:239:LYS:HD2	1.95	0.48
1:C:388:LEU:O	1:C:392:ILE:HG13	2.13	0.48
1:F:143:ASP:O	1:F:147:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:TYR:CE2	1:H:497:LEU:HA	2.49	0.48
1:F:113:LEU:HB3	1:F:114:PRO:HD2	1.96	0.48
1:G:352:ALA:HB2	1:G:405:ASP:HB2	1.96	0.48
1:H:507:SER:O	1:H:510:GLN:HB2	2.14	0.48
1:E:345:LYS:HG2	1:E:364:GLU:HG3	1.95	0.48
1:B:388:LEU:O	1:B:392:ILE:HG13	2.14	0.48
1:G:65:ILE:HD12	1:G:65:ILE:HA	1.64	0.48
1:F:158:PHE:CD1	1:F:319:PRO:HG3	2.49	0.47
1:G:146:ILE:O	1:G:149:MET:HB2	2.14	0.47
1:G:149:MET:HG2	1:G:184:ALA:HB1	1.96	0.47
1:H:139:PRO:CB	1:H:145:TRP:HB2	2.44	0.47
1:F:91:ARG:O	1:F:92:ILE:HD13	2.14	0.47
1:E:431:THR:O	1:E:435:PRO:HG3	2.14	0.47
1:A:395:LEU:HD22	1:A:400:MET:CE	2.44	0.47
1:H:383:ASN:O	1:H:387:ILE:HB	2.14	0.47
1:G:21:GLY:HA2	1:G:462:PHE:CE1	2.48	0.47
1:G:401:LEU:HB3	1:G:405:ASP:HB2	1.96	0.47
1:E:387:ILE:HG23	1:E:388:LEU:N	2.28	0.47
1:F:447:ARG:O	1:F:451:TRP:HA	2.14	0.47
1:D:72:PHE:CE2	1:D:76:LEU:HD11	2.48	0.47
1:C:250:LYS:HD3	1:C:262:TYR:O	2.14	0.47
1:E:272:ASP:N	1:E:272:ASP:OD1	2.47	0.47
1:C:420:PRO:O	1:C:422:PRO:HD3	2.14	0.47
1:G:433:ILE:O	1:G:436:LYS:HB2	2.14	0.47
1:F:402:LYS:HE3	1:F:404:THR:OG1	2.13	0.47
1:C:57:LEU:CD2	1:C:338:ASN:HA	2.43	0.47
1:G:212:PHE:CD2	1:G:213:PRO:HD2	2.49	0.47
1:B:249:ASN:O	1:B:251:THR:HG23	2.14	0.47
1:F:173:LYS:HA	1:F:424:LEU:HD11	1.95	0.47
1:H:43:PRO:HG2	1:H:223:ILE:HD13	1.95	0.47
1:E:391:CYS:O	1:E:395:LEU:HG	2.14	0.47
1:E:134:VAL:O	1:E:134:VAL:CG1	2.61	0.47
1:H:149:MET:SD	1:H:184:ALA:O	2.72	0.47
1:A:115:LYS:O	1:A:118:GLN:HB2	2.15	0.47
1:F:126:ILE:O	1:F:130:LEU:HG	2.14	0.47
1:A:126:ILE:CD1	1:G:189:LYS:HG2	2.45	0.47
1:G:296:HIS:HB2	1:G:374:VAL:HB	1.95	0.47
1:G:350:GLN:OE1	1:G:354:GLY:HA2	2.15	0.47
1:A:199:LYS:HD2	1:A:200:THR:N	2.30	0.47
1:F:56:PHE:CD2	1:F:409:SER:HB3	2.49	0.47
2:A:601:FAD:C2'	2:A:601:FAD:H9	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:ILE:N	1:E:154:ILE:HD13	2.22	0.47
1:E:175:GLN:OE1	1:E:178:TRP:HD1	1.97	0.47
1:C:69:TYR:CD1	1:C:463:MET:HG3	2.48	0.47
1:F:455:VAL:HA	1:F:460:HIS:HD1	1.79	0.47
1:A:351:LEU:HB2	1:A:355:SER:OG	2.14	0.47
1:E:19:GLY:O	1:E:22:ALA:HB3	2.15	0.47
1:B:179:LEU:HD23	1:B:183:VAL:HG21	1.96	0.47
1:G:447:ARG:NH1	2:G:601:FAD:H1'1	2.28	0.47
1:H:292:TYR:HB3	1:H:451:TRP:CZ2	2.49	0.47
1:B:175:GLN:HE22	1:B:177:ALA:HB3	1.80	0.47
1:E:63:HIS:CE1	2:E:601:FAD:N10	2.82	0.47
1:G:302:VAL:HA	1:G:406:GLU:O	2.14	0.47
1:G:342:ALA:O	1:G:365:GLY:O	2.32	0.47
1:A:331:PHE:HB3	1:A:369:SER:HB3	1.96	0.47
1:C:150:MET:HE3	1:C:159:MET:HG3	1.97	0.47
1:C:106:PHE:C	1:C:106:PHE:CD2	2.88	0.47
1:G:24:LYS:HA	1:G:24:LYS:HD3	1.67	0.47
1:H:62:GLY:O	2:H:601:FAD:O4	2.31	0.47
1:D:420:PRO:O	1:D:422:PRO:HD3	2.14	0.47
1:C:175:GLN:NE2	1:C:177:ALA:HB3	2.30	0.47
1:B:175:GLN:NE2	1:B:177:ALA:HB3	2.30	0.47
1:F:51:VAL:HG12	1:F:52:THR:O	2.14	0.47
1:E:56:PHE:HE1	1:E:339:GLN:HB3	1.75	0.47
1:E:179:LEU:CD2	1:E:179:LEU:N	2.77	0.47
1:G:351:LEU:HB2	1:G:355:SER:H	1.78	0.47
1:B:207:ASN:O	1:B:208:ALA:C	2.53	0.47
1:B:108:ASN:HB2	1:B:194:ASN:OD1	2.14	0.47
1:A:455:VAL:HG21	1:A:480:THR:O	2.15	0.47
1:G:165:LYS:HD3	1:G:318:PHE:O	2.14	0.47
1:B:306:ARG:HA	1:B:307:PRO:HD3	1.79	0.47
1:F:286:LEU:O	1:F:289:GLN:HB2	2.14	0.47
1:F:109:ASN:N	1:F:109:ASN:ND2	2.63	0.47
1:G:460:HIS:NE2	1:G:488:ASN:OD1	2.47	0.47
1:H:418:GLY:O	1:H:419:TYR:HD1	1.96	0.47
1:B:192:THR:OG1	1:B:193:THR:N	2.47	0.47
1:E:63:HIS:CD2	1:E:63:HIS:N	2.81	0.47
1:H:332:SER:HA	1:H:339:GLN:HE22	1.75	0.47
1:H:337:TYR:N	1:H:337:TYR:HD1	2.12	0.47
1:A:178:TRP:CB	1:A:454:GLU:CG	2.92	0.47
1:F:265:LEU:O	1:F:442:ILE:HA	2.14	0.47
1:B:57:LEU:CD2	1:B:338:ASN:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:72:PHE:CE1	1:H:459:ASP:HA	2.50	0.47
1:B:87:TYR:HB3	1:B:89:HIS:HE1	1.80	0.47
1:C:483:TYR:N	1:C:484:PRO:HD3	2.30	0.47
1:E:47:ALA:HB1	1:E:222:TRP:NE1	2.30	0.47
1:H:187:ASN:OD1	1:H:190:ALA:CB	2.63	0.47
1:F:244:LYS:HG2	1:F:245:VAL:N	2.30	0.47
1:H:221:ILE:O	1:H:224:ALA:HB3	2.15	0.47
1:D:103:PRO:HB2	1:D:109:ASN:OD1	2.15	0.47
1:C:395:LEU:HD22	1:C:400:MET:CE	2.45	0.47
1:B:130:LEU:HD23	1:H:130:LEU:CD2	2.44	0.47
1:D:417:HIS:HB3	1:D:448:PHE:CZ	2.49	0.47
1:C:269:MET:HG2	1:C:274:LEU:HD22	1.96	0.47
1:G:426:ARG:O	1:G:430:LEU:HG	2.15	0.47
1:D:168:ALA:HB1	1:D:377:SER:HB3	1.97	0.47
1:A:344:LYS:HD2	1:A:345:LYS:H	1.79	0.47
1:E:82:LYS:HB2	1:E:85:ASP:OD2	2.15	0.47
1:B:107:GLN:CD	1:B:107:GLN:H	2.17	0.47
1:G:420:PRO:HB2	1:G:451:TRP:CD1	2.50	0.47
1:E:63:HIS:ND1	2:E:601:FAD:C10	2.78	0.47
1:D:17:PRO:HG2	2:D:601:FAD:H4'	1.96	0.47
1:E:274:LEU:O	1:E:278:MET:HG2	2.13	0.47
1:E:6:ILE:O	1:E:260:ILE:HA	2.14	0.47
1:H:64:VAL:HG22	1:H:210:PHE:CE1	2.49	0.47
1:H:175:GLN:HG3	1:H:178:TRP:CD1	2.50	0.47
1:F:139:PRO:HA	1:F:144:GLU:OE2	2.14	0.47
1:C:437:LEU:HD12	1:C:444:SER:HB2	1.96	0.47
1:F:22:ALA:O	1:F:26:LEU:HB2	2.14	0.47
1:B:17:PRO:O	1:B:462:PHE:HA	2.15	0.47
1:H:467:GLU:OE1	1:H:479:LEU:N	2.48	0.47
1:E:158:PHE:O	1:E:161:PRO:HG2	2.15	0.47
1:H:96:ARG:HB2	1:H:101:TRP:CZ3	2.50	0.47
1:D:57:LEU:HD13	1:D:338:ASN:C	2.35	0.47
1:B:346:LEU:HD13	1:B:408:VAL:CG1	2.45	0.47
1:B:242:VAL:HA	1:B:254:LEU:CD2	2.45	0.47
1:A:494:GLU:HG2	1:E:477:VAL:HB	1.96	0.47
1:E:508:LYS:HG3	1:E:509:ALA:N	2.29	0.47
1:H:65:ILE:O	1:H:65:ILE:HG22	2.14	0.47
1:C:119:VAL:HA	1:E:196:ILE:CD1	2.44	0.46
1:E:207:ASN:HB3	1:E:315:TRP:HH2	1.78	0.46
1:A:136:ASN:OD1	1:A:136:ASN:N	2.33	0.46
1:D:395:LEU:HD22	1:D:400:MET:CE	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LEU:HA	1:F:405:ASP:O	2.14	0.46
1:G:210:PHE:N	1:G:210:PHE:HD2	2.13	0.46
1:D:278:MET:HE2	1:D:442:ILE:HD12	1.96	0.46
1:B:473:VAL:O	1:F:499:ASP:HB3	2.16	0.46
1:A:113:LEU:O	1:A:118:GLN:NE2	2.34	0.46
1:A:119:VAL:HG22	1:G:193:THR:HG22	1.96	0.46
1:B:178:TRP:CB	1:B:454:GLU:CG	2.92	0.46
1:A:358:GLN:CD	1:A:358:GLN:N	2.64	0.46
1:H:326:TYR:CE2	1:H:375:SER:HB3	2.50	0.46
1:C:335:SER:HB3	1:C:338:ASN:OD1	2.14	0.46
1:C:39:SER:CB	1:C:241:LYS:HG2	2.45	0.46
1:F:95:VAL:HG23	1:F:102:VAL:O	2.16	0.46
1:G:106:PHE:CZ	1:G:113:LEU:HD11	2.50	0.46
1:B:287:THR:O	1:B:290:LEU:HD12	2.16	0.46
1:E:139:PRO:HA	1:E:144:GLU:OE2	2.16	0.46
1:G:425:GLU:CD	1:G:425:GLU:N	2.69	0.46
1:A:106:PHE:CD2	1:A:106:PHE:C	2.87	0.46
1:E:17:PRO:C	1:E:462:PHE:HA	2.35	0.46
1:F:467:GLU:HG2	1:F:495:ARG:HH22	1.79	0.46
1:E:275:ALA:HB1	1:E:284:VAL:HG22	1.97	0.46
1:H:58:TYR:CZ	1:H:299:GLY:HA3	2.50	0.46
1:A:207:ASN:O	1:A:208:ALA:C	2.53	0.46
1:C:234:THR:HB	1:C:236:PHE:CZ	2.51	0.46
1:G:323:CYS:HB2	1:G:325:PHE:CE1	2.49	0.46
1:D:304:GLY:O	1:D:368:TRP:CD1	2.68	0.46
1:E:70:LYS:HB3	1:E:496:ARG:NH1	2.27	0.46
1:E:10:VAL:O	1:E:34:TRP:HA	2.15	0.46
1:E:457:ASN:HB3	2:E:601:FAD:N1	2.31	0.46
1:A:46:LEU:O	1:A:63:HIS:HE1	1.98	0.46
1:C:196:ILE:HG21	1:E:119:VAL:CG2	2.44	0.46
1:B:350:GLN:NE2	1:B:351:LEU:O	2.49	0.46
1:E:402:LYS:HE3	1:E:404:THR:OG1	2.15	0.46
1:D:94:TYR:CD1	1:D:101:TRP:HB3	2.51	0.46
1:H:376:GLU:CG	1:H:382:VAL:HG13	2.35	0.46
1:D:175:GLN:HE22	1:D:177:ALA:HB3	1.80	0.46
1:G:351:LEU:CD1	1:G:404:THR:HA	2.46	0.46
1:F:376:GLU:HB2	1:F:382:VAL:CG1	2.45	0.46
1:A:417:HIS:HB3	1:A:448:PHE:CZ	2.50	0.46
1:A:106:PHE:C	1:A:106:PHE:HD2	2.19	0.46
3:C:602:GDU:O2A	3:C:602:GDU:H4D	2.16	0.46
1:E:167:TRP:O	1:E:169:VAL:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:171:THR:HG22	1:G:174:MET:HE3	1.97	0.46
1:E:56:PHE:CE2	1:E:409:SER:HB3	2.50	0.46
1:E:454:GLU:CD	1:E:454:GLU:H	2.12	0.46
1:G:70:LYS:HB2	1:G:493:THR:HA	1.98	0.46
1:G:499:ASP:HB2	1:G:502:GLN:OE1	2.16	0.46
1:G:499:ASP:O	1:G:502:GLN:N	2.48	0.46
1:H:70:LYS:HA	1:H:70:LYS:HD2	1.62	0.46
1:H:210:PHE:HD2	1:H:210:PHE:N	2.13	0.46
1:H:367:TYR:HD1	1:H:408:VAL:HG21	1.80	0.46
1:G:210:PHE:N	1:G:210:PHE:CD2	2.83	0.46
1:A:94:TYR:CD1	1:A:101:TRP:HB3	2.50	0.46
1:G:292:TYR:HB3	1:G:451:TRP:CZ2	2.50	0.46
1:E:167:TRP:CG	1:E:174:MET:HE3	2.51	0.46
1:E:56:PHE:CD2	1:E:409:SER:HB3	2.51	0.46
1:D:207:ASN:O	1:D:208:ALA:C	2.54	0.46
1:D:304:GLY:O	1:D:368:TRP:HD1	1.97	0.46
1:D:473:VAL:HG12	1:H:501:ALA:HA	1.98	0.46
1:H:469:VAL:HA	1:H:472:ILE:HD12	1.98	0.46
1:H:2:THR:OG1	1:H:3:HIS:N	2.47	0.46
1:A:232:GLU:CD	1:A:232:GLU:H	2.19	0.46
1:E:467:GLU:CG	1:E:495:ARG:HH12	2.29	0.46
1:D:303:ARG:NH1	1:D:348:THR:OG1	2.49	0.46
1:D:303:ARG:NH2	1:D:363:LYS:O	2.43	0.46
1:E:38:ASP:HB3	1:E:236:PHE:HD1	1.79	0.46
1:F:332:SER:HB3	1:F:369:SER:H	1.80	0.46
1:G:143:ASP:HA	1:G:146:ILE:CD1	2.43	0.46
1:A:193:THR:O	1:A:196:ILE:HB	2.15	0.46
1:H:197:LEU:C	1:H:199:LYS:N	2.67	0.46
1:C:395:LEU:HD22	1:C:400:MET:HE2	1.97	0.46
1:E:250:LYS:O	1:E:261:GLY:HA2	2.16	0.46
1:B:45:GLY:HA3	2:B:601:FAD:O1A	2.16	0.46
1:G:467:GLU:OE1	1:G:480:THR:OG1	2.27	0.46
1:G:196:ILE:HG22	1:G:197:LEU:N	2.31	0.46
1:H:419:TYR:N	1:H:419:TYR:CD1	2.84	0.46
1:H:63:HIS:HB2	1:H:218:THR:HG21	1.97	0.46
1:E:63:HIS:CE1	2:E:601:FAD:C9	2.99	0.46
1:H:109:ASN:C	1:H:111:SER:N	2.69	0.46
1:E:69:TYR:CE2	1:E:463:MET:HG3	2.51	0.46
1:C:398:THR:HB	1:C:400:MET:CG	2.46	0.46
1:G:25:ARG:NH1	1:G:470:ASP:OD2	2.49	0.46
1:G:28:GLN:NE2	1:G:497:LEU:O	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:MET:CE	1:A:186:PRO:HB2	2.44	0.46
1:B:60:VAL:O	1:B:61:GLY:O	2.34	0.46
1:B:57:LEU:CD1	1:B:57:LEU:N	2.79	0.46
1:C:344:LYS:HD2	1:C:345:LYS:H	1.79	0.46
1:B:152:THR:HG22	1:B:156:ASP:OD2	2.16	0.46
1:G:44:GLY:HA2	1:G:222:TRP:CD1	2.51	0.46
1:G:460:HIS:CE1	1:G:488:ASN:OD1	2.68	0.46
1:B:136:ASN:ND2	1:F:133:ARG:HE	2.14	0.46
1:F:9:ASP:H	1:F:33:SER:HG	1.55	0.46
1:D:38:ASP:OD1	2:D:601:FAD:H1B	2.15	0.46
1:B:325:PHE:CZ	1:B:395:LEU:HD23	2.50	0.46
1:E:349:MET:O	1:E:350:GLN:HB3	2.16	0.46
1:H:192:THR:OG1	1:H:193:THR:N	2.49	0.46
1:F:12:VAL:O	1:F:36:ILE:HA	2.15	0.46
1:B:455:VAL:O	1:B:460:HIS:CB	2.62	0.46
1:A:398:THR:HB	1:A:400:MET:HG2	1.98	0.46
1:H:178:TRP:N	1:H:178:TRP:CD1	2.84	0.46
1:E:71:TYR:HB2	1:E:495:ARG:O	2.16	0.45
1:F:18:THR:O	1:F:465:GLY:HA3	2.16	0.45
1:E:143:ASP:OD2	1:E:171:THR:OG1	2.30	0.45
1:H:299:GLY:HA2	1:H:370:ILE:O	2.16	0.45
1:A:204:TRP:CE3	1:A:205:GLY:N	2.85	0.45
1:G:103:PRO:HB2	1:G:202:GLY:HA3	1.97	0.45
1:E:430:LEU:HD23	1:E:430:LEU:HA	1.73	0.45
1:C:244:LYS:HG2	1:C:245:VAL:N	2.30	0.45
1:B:500:GLY:HA3	1:F:472:ILE:O	2.16	0.45
1:B:443:TRP:CE3	1:B:443:TRP:N	2.84	0.45
1:F:64:VAL:CG1	1:F:65:ILE:N	2.79	0.45
1:G:92:ILE:HB	1:G:314:CYS:H	1.81	0.45
1:H:126:ILE:HA	1:H:188:LEU:HD11	1.98	0.45
1:E:306:ARG:NH1	1:E:333:ASN:OD1	2.49	0.45
1:A:301:GLY:HA3	1:A:409:SER:CB	2.46	0.45
1:A:483:TYR:N	1:A:484:PRO:HD3	2.30	0.45
1:C:100:GLN:HA	1:C:100:GLN:OE1	2.17	0.45
1:G:273:PHE:N	1:G:273:PHE:CD1	2.81	0.45
1:F:142:PHE:HB2	1:F:174:MET:HB2	1.96	0.45
1:G:271:VAL:HB	1:G:449:GLY:O	2.16	0.45
1:G:54:GLU:HB3	1:G:346:LEU:CD1	2.45	0.45
1:A:350:GLN:HE21	1:A:350:GLN:HB2	1.52	0.45
1:E:187:ASN:CG	1:E:189:LYS:HB2	2.36	0.45
1:H:196:ILE:HG22	1:H:197:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:HG2	1:F:92:ILE:N	2.31	0.45
1:H:401:LEU:HB3	1:H:405:ASP:HB2	1.99	0.45
1:E:66:PHE:HB3	1:E:206:PRO:O	2.15	0.45
1:C:469:VAL:O	1:C:472:ILE:N	2.48	0.45
1:A:150:MET:HG2	1:A:154:ILE:HG21	1.97	0.45
1:G:12:VAL:HA	1:G:266:VAL:O	2.17	0.45
1:F:22:ALA:HA	1:F:469:VAL:HG21	1.97	0.45
1:G:69:TYR:HD1	1:G:492:ASN:HB2	1.81	0.45
1:H:292:TYR:CZ	1:H:417:HIS:CE1	3.04	0.45
1:H:417:HIS:HB3	1:H:448:PHE:CD2	2.50	0.45
1:G:207:ASN:OD1	1:G:208:ALA:N	2.49	0.45
1:H:44:GLY:HA2	1:H:222:TRP:CD1	2.52	0.45
1:E:51:VAL:HG22	1:E:57:LEU:HG	1.97	0.45
1:G:306:ARG:HA	1:G:307:PRO:HD3	1.55	0.45
1:A:457:ASN:O	1:A:460:HIS:HB2	2.16	0.45
1:C:480:THR:HA	1:C:487:VAL:HG11	1.97	0.45
1:A:160:ARG:N	1:A:161:PRO:HD2	2.31	0.45
1:B:443:TRP:CD1	1:B:445:ARG:NH2	2.84	0.45
1:G:156:ASP:HB2	1:G:157:LEU:HD12	1.98	0.45
1:H:106:PHE:CZ	1:H:113:LEU:HD11	2.51	0.45
1:F:17:PRO:O	1:F:462:PHE:CD1	2.69	0.45
1:A:110:ILE:CA	1:A:113:LEU:HD12	2.42	0.45
1:F:336:PRO:HG2	1:F:337:TYR:CE1	2.52	0.45
1:A:6:ILE:N	1:A:6:ILE:HD13	2.32	0.45
1:A:296:HIS:CE1	1:A:382:VAL:HG21	2.50	0.45
1:E:264:LYS:HD3	1:E:472:ILE:HG23	1.98	0.45
1:G:483:TYR:N	1:G:484:PRO:HD3	2.31	0.45
2:G:601:FAD:O1A	2:G:601:FAD:O5'	2.30	0.45
1:A:199:LYS:HB3	1:A:199:LYS:HE2	1.67	0.45
1:H:464:LEU:HD21	1:H:481:LEU:N	2.32	0.45
1:D:242:VAL:HG23	2:D:601:FAD:N1A	2.31	0.45
1:C:196:ILE:HD12	1:E:119:VAL:HG22	1.98	0.45
1:H:181:GLU:O	1:H:181:GLU:HG3	2.16	0.45
1:E:499:ASP:O	1:E:503:VAL:HG23	2.16	0.45
1:G:70:LYS:HA	1:G:70:LYS:HD2	1.77	0.45
1:E:265:LEU:O	1:E:442:ILE:HA	2.17	0.45
1:A:325:PHE:CA	1:A:374:VAL:HG22	2.46	0.45
1:C:301:GLY:HA3	1:C:409:SER:CB	2.45	0.45
1:C:307:PRO:HB2	1:C:309:ARG:HG2	1.99	0.45
1:H:486:PHE:CE2	1:H:490:ARG:HD2	2.52	0.45
1:B:344:LYS:HD2	1:B:345:LYS:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:219:GLY:O	1:H:223:ILE:HG12	2.16	0.45
1:F:286:LEU:HD21	1:F:436:LYS:HE3	1.98	0.45
1:C:304:GLY:O	1:C:368:TRP:HD1	1.99	0.45
1:B:106:PHE:C	1:B:106:PHE:CD2	2.90	0.45
1:E:70:LYS:NZ	1:E:73:ASP:HB2	2.32	0.45
1:C:455:VAL:HG11	1:C:464:LEU:HD11	1.99	0.45
1:C:19:GLY:H	1:C:268:THR:HG21	1.81	0.45
1:D:395:LEU:HA	1:D:400:MET:HG3	1.97	0.45
1:F:504:PHE:CD1	1:F:504:PHE:N	2.82	0.45
1:C:272:ASP:N	1:C:272:ASP:OD1	2.48	0.45
1:E:70:LYS:O	1:E:70:LYS:HE3	2.17	0.45
1:H:69:TYR:HD1	1:H:492:ASN:HB2	1.80	0.45
1:C:192:THR:OG1	1:C:193:THR:N	2.49	0.45
1:H:130:LEU:O	1:H:133:ARG:CB	2.63	0.45
1:F:207:ASN:HB3	1:F:315:TRP:CZ2	2.52	0.45
1:H:181:GLU:OE1	1:H:181:GLU:CA	2.62	0.45
1:B:119:VAL:HG13	1:H:193:THR:CG2	2.47	0.45
1:B:350:GLN:NE2	1:B:354:GLY:HA2	2.28	0.45
1:E:107:GLN:O	1:E:110:ILE:HG22	2.16	0.45
1:G:72:PHE:CE1	1:G:459:ASP:HA	2.51	0.45
1:D:335:SER:OG	1:D:336:PRO:HD2	2.17	0.45
1:H:210:PHE:HZ	1:H:334:TYR:CE1	2.34	0.45
1:F:269:MET:HE3	1:F:273:PHE:HB3	1.99	0.45
1:C:96:ARG:O	1:C:319:PRO:HD2	2.16	0.45
1:A:312:ASP:OD1	1:A:312:ASP:N	2.44	0.45
1:E:318:PHE:CZ	1:E:325:PHE:HE1	2.35	0.45
1:G:150:MET:CG	1:G:154:ILE:HB	2.36	0.45
1:E:91:ARG:O	1:E:92:ILE:HD13	2.16	0.45
1:H:351:LEU:O	1:H:354:GLY:N	2.43	0.45
1:C:395:LEU:HA	1:C:400:MET:HG3	1.99	0.45
1:G:130:LEU:O	1:G:133:ARG:N	2.50	0.45
1:E:109:ASN:ND2	1:E:109:ASN:N	2.62	0.45
1:D:194:ASN:HD22	1:D:194:ASN:HA	1.55	0.45
1:C:346:LEU:HD13	1:C:408:VAL:CG1	2.47	0.45
1:H:353:ASP:HB3	1:H:403:PRO:CB	2.46	0.45
1:A:150:MET:HE3	1:A:159:MET:HG3	1.98	0.45
1:H:421:THR:HA	1:H:422:PRO:HD3	1.74	0.45
1:G:86:TRP:HA	1:G:86:TRP:CE3	2.52	0.45
1:D:35:MET:HE1	1:D:235:ARG:HG3	1.98	0.45
1:F:209:THR:O	1:F:210:PHE:HB3	2.17	0.45
1:H:273:PHE:CD1	1:H:273:PHE:N	2.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:VAL:HA	1:E:326:TYR:CD2	2.52	0.45
1:E:325:PHE:HA	1:E:374:VAL:CG2	2.47	0.45
1:H:61:GLY:HA3	2:H:601:FAD:H6	1.98	0.45
1:D:175:GLN:NE2	1:D:177:ALA:HB3	2.32	0.45
1:B:125:MET:HG2	1:B:188:LEU:HD13	1.99	0.45
1:C:425:GLU:H	1:C:425:GLU:CD	2.20	0.45
1:B:116:GLU:O	1:B:119:VAL:HB	2.17	0.45
1:D:115:LYS:HB3	1:F:197:LEU:CD2	2.46	0.45
1:F:436:LYS:O	1:F:439:ASP:HB2	2.16	0.45
1:H:187:ASN:OD1	1:H:190:ALA:HB2	2.17	0.45
1:G:30:ASP:O	1:G:30:ASP:OD1	2.35	0.45
1:E:235:ARG:HG2	1:E:239:LYS:HD2	1.98	0.45
1:D:70:LYS:HA	1:D:70:LYS:HD2	1.51	0.45
1:B:28:GLN:NE2	1:B:497:LEU:O	2.50	0.45
1:A:339:GLN:N	1:A:339:GLN:CD	2.71	0.44
1:H:443:TRP:N	1:H:443:TRP:HE3	2.15	0.44
1:E:332:SER:CB	1:E:369:SER:H	2.29	0.44
1:H:104:TYR:CG	1:H:105:PRO:HA	2.52	0.44
1:D:323:CYS:HB2	1:D:325:PHE:CE2	2.52	0.44
1:D:307:PRO:HD2	1:D:310:ILE:HD12	1.98	0.44
1:B:304:GLY:O	1:B:368:TRP:CD1	2.70	0.44
1:H:134:VAL:CG1	1:H:134:VAL:O	2.64	0.44
1:C:376:GLU:HA	1:C:380:LYS:O	2.17	0.44
1:C:434:LEU:HA	1:C:434:LEU:HD23	1.84	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CD2	2.52	0.44
1:G:417:HIS:HB3	1:G:448:PHE:CZ	2.51	0.44
1:E:163:ASN:HA	1:E:166:VAL:CG1	2.46	0.44
1:E:63:HIS:H	1:E:63:HIS:CD2	2.33	0.44
1:G:139:PRO:HA	1:G:144:GLU:OE2	2.17	0.44
1:G:312:ASP:N	1:G:312:ASP:OD1	2.37	0.44
1:C:91:ARG:O	1:C:92:ILE:HD13	2.17	0.44
1:E:187:ASN:O	1:E:191:VAL:HG23	2.18	0.44
1:C:19:GLY:O	1:C:22:ALA:HB3	2.17	0.44
1:D:115:LYS:HD3	1:F:197:LEU:HA	1.98	0.44
1:A:106:PHE:HD2	1:A:106:PHE:O	2.01	0.44
1:B:138:LYS:HB2	1:B:138:LYS:HE3	1.86	0.44
1:E:385:GLU:HG2	1:E:385:GLU:H	1.47	0.44
1:F:167:TRP:CG	1:F:174:MET:HE1	2.53	0.44
1:E:10:VAL:HG13	1:E:264:LYS:HB2	2.00	0.44
1:E:445:ARG:CZ	1:E:481:LEU:HD22	2.46	0.44
1:E:104:TYR:CE1	3:E:602:GDU:H5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:299:GLY:HA2	1:G:371:MET:HA	1.98	0.44
1:G:348:THR:HG21	1:G:406:GLU:HG2	2.00	0.44
1:H:107:GLN:CD	1:H:107:GLN:N	2.66	0.44
1:C:325:PHE:HA	1:C:374:VAL:HG22	1.98	0.44
1:G:283:LEU:HD22	1:G:433:ILE:HG23	1.99	0.44
1:G:254:LEU:HB2	1:G:258:THR:HB	1.98	0.44
1:D:398:THR:O	1:D:399:GLU:HB2	2.17	0.44
1:A:57:LEU:HD13	1:A:338:ASN:C	2.38	0.44
1:H:210:PHE:N	1:H:210:PHE:CD2	2.84	0.44
1:F:307:PRO:HD3	1:F:368:TRP:CE2	2.52	0.44
1:B:6:ILE:O	1:B:260:ILE:HA	2.17	0.44
1:C:299:GLY:HA2	1:C:370:ILE:O	2.17	0.44
1:D:138:LYS:HA	1:D:139:PRO:HD3	1.83	0.44
1:F:134:VAL:CG1	1:F:134:VAL:O	2.65	0.44
1:E:467:GLU:HG2	1:E:495:ARG:CZ	2.48	0.44
1:F:151:GLY:C	1:F:154:ILE:HG12	2.36	0.44
1:H:276:GLU:O	1:H:279:ASN:N	2.48	0.44
1:E:159:MET:HE3	3:E:602:GDU:C2	2.47	0.44
1:G:148:ARG:O	1:G:186:PRO:HD3	2.18	0.44
1:A:178:TRP:CZ3	1:A:179:LEU:HD23	2.52	0.44
1:A:91:ARG:O	1:A:92:ILE:HD13	2.18	0.44
1:C:350:GLN:HE21	1:C:350:GLN:HB2	1.57	0.44
1:G:341:GLU:CG	1:G:343:SER:H	2.27	0.44
1:H:9:ASP:OD1	1:H:33:SER:N	2.49	0.44
1:D:108:ASN:HB2	1:D:194:ASN:OD1	2.18	0.44
1:B:58:TYR:HA	1:B:331:PHE:CE2	2.47	0.44
1:C:106:PHE:HD2	1:C:106:PHE:C	2.20	0.44
1:H:271:VAL:HB	1:H:449:GLY:O	2.17	0.44
1:E:318:PHE:CE2	1:E:398:THR:HG21	2.52	0.44
1:F:125:MET:CG	1:F:188:LEU:HD13	2.46	0.44
1:H:455:VAL:HG21	1:H:480:THR:O	2.17	0.44
1:E:167:TRP:CG	1:E:174:MET:CE	3.01	0.44
1:H:152:THR:O	1:H:156:ASP:CG	2.55	0.44
1:H:158:PHE:O	1:H:161:PRO:HD2	2.17	0.44
1:E:110:ILE:CG2	1:E:195:VAL:HG22	2.47	0.44
1:F:275:ALA:HB1	1:F:284:VAL:HG22	1.99	0.44
1:C:42:THR:HG22	1:C:223:ILE:HD11	1.98	0.44
1:C:57:LEU:HD13	1:C:338:ASN:C	2.38	0.44
1:H:65:ILE:HD12	1:H:65:ILE:HA	1.61	0.44
1:E:286:LEU:O	1:E:289:GLN:HB2	2.18	0.44
1:A:5:ASP:N	1:A:259:THR:OG1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:TYR:CE1	1:E:299:GLY:HA3	2.52	0.44
1:C:194:ASN:HD22	1:C:194:ASN:HA	1.59	0.44
1:F:70:LYS:CB	1:F:496:ARG:HH12	2.29	0.44
1:F:162:TYR:O	1:F:166:VAL:CG1	2.65	0.44
1:A:103:PRO:HG2	1:A:109:ASN:OD1	2.17	0.44
1:A:38:ASP:OD2	1:A:40:ASN:CB	2.65	0.44
1:E:425:GLU:CD	1:E:425:GLU:N	2.70	0.44
1:F:443:TRP:HE3	1:F:443:TRP:H	1.64	0.44
1:F:137:THR:C	1:F:148:ARG:HH12	2.20	0.44
1:H:223:ILE:HD13	1:H:223:ILE:N	2.33	0.44
1:H:434:LEU:HB2	1:H:435:PRO:HD3	2.00	0.44
1:F:310:ILE:HG22	1:F:311:GLY:N	2.32	0.44
1:C:297:VAL:O	1:C:298:ILE:HD13	2.18	0.44
1:D:346:LEU:HD13	1:D:408:VAL:HG13	1.99	0.44
1:G:18:THR:CB	2:G:601:FAD:O2P	2.66	0.44
1:E:104:TYR:CE1	3:E:602:GDU:C5	2.94	0.44
1:A:447:ARG:HD2	2:A:601:FAD:H3'	2.00	0.44
1:H:296:HIS:HB2	1:H:374:VAL:HB	1.98	0.44
1:C:193:THR:O	1:C:197:LEU:HG	2.17	0.44
1:B:119:VAL:HG13	1:H:193:THR:HG22	1.99	0.44
1:E:336:PRO:HG2	1:E:337:TYR:CE1	2.53	0.44
1:F:294:SER:CB	1:F:414:ARG:NH2	2.80	0.44
1:F:298:ILE:O	1:F:298:ILE:HG22	2.16	0.44
1:C:437:LEU:CD1	1:C:444:SER:HB2	2.48	0.44
1:G:108:ASN:OD1	1:G:108:ASN:N	2.49	0.44
1:B:150:MET:HE3	1:B:159:MET:HG3	1.99	0.44
1:G:204:TRP:O	1:G:208:ALA:HB3	2.18	0.44
1:G:348:THR:HB	1:G:357:PRO:HB3	2.00	0.44
1:D:455:VAL:O	1:D:460:HIS:CB	2.64	0.44
1:F:107:GLN:NE2	1:F:108:ASN:OD1	2.51	0.44
1:E:306:ARG:O	1:E:306:ARG:HG2	2.18	0.44
1:E:109:ASN:HD22	1:E:109:ASN:N	2.16	0.44
1:F:382:VAL:HG23	1:F:383:ASN:N	2.32	0.44
1:A:398:THR:O	1:A:399:GLU:HB2	2.18	0.44
1:C:249:ASN:O	1:C:251:THR:HG23	2.17	0.44
1:E:24:LYS:HA	1:E:24:LYS:HD3	1.73	0.44
1:D:296:HIS:CE1	1:D:382:VAL:HG21	2.52	0.44
1:F:18:THR:HG23	1:F:464:LEU:HB2	1.98	0.44
1:A:183:VAL:HG22	3:A:602:GDU:C1D	2.48	0.44
1:H:443:TRP:N	1:H:443:TRP:CE3	2.86	0.44
1:H:296:HIS:ND1	1:H:412:HIS:HE1	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:303:ARG:HH21	1:E:363:LYS:HB2	1.82	0.44
1:B:350:GLN:HE21	1:B:350:GLN:HB2	1.51	0.44
1:C:264:LYS:HD2	1:C:443:TRP:CH2	2.53	0.44
1:G:160:ARG:HB2	1:G:161:PRO:CD	2.48	0.44
1:B:433:ILE:O	1:B:436:LYS:HB2	2.17	0.44
1:B:469:VAL:O	1:B:473:VAL:HG23	2.18	0.44
1:B:402:LYS:HB3	1:B:404:THR:HG23	2.00	0.44
1:G:5:ASP:C	1:G:6:ILE:HG12	2.37	0.44
1:H:5:ASP:C	1:H:6:ILE:HG12	2.38	0.44
1:D:384:GLN:HG2	1:D:384:GLN:H	1.65	0.44
1:A:425:GLU:CD	1:A:425:GLU:H	2.20	0.44
1:G:445:ARG:HH11	1:G:481:LEU:HD22	1.81	0.43
1:A:199:LYS:HD2	1:A:200:THR:H	1.83	0.43
1:H:15:ALA:HB2	1:H:38:ASP:HB2	2.00	0.43
1:H:57:LEU:HD11	1:H:337:TYR:O	2.17	0.43
1:E:349:MET:O	1:E:350:GLN:CB	2.66	0.43
1:A:455:VAL:O	1:A:460:HIS:CB	2.63	0.43
1:C:46:LEU:HB2	2:C:601:FAD:O4'	2.18	0.43
1:A:194:ASN:HD22	1:A:194:ASN:HA	1.61	0.43
1:E:244:LYS:HB3	1:E:244:LYS:HE3	1.74	0.43
1:G:65:ILE:O	1:G:65:ILE:HG22	2.18	0.43
1:C:67:SER:HA	1:C:459:ASP:OD2	2.17	0.43
1:A:499:ASP:O	1:A:503:VAL:HG23	2.18	0.43
1:H:108:ASN:N	1:H:108:ASN:OD1	2.51	0.43
1:C:407:ILE:O	1:C:407:ILE:HG22	2.18	0.43
1:F:109:ASN:HD22	1:F:109:ASN:N	2.16	0.43
1:B:110:ILE:CA	1:B:113:LEU:HD12	2.37	0.43
1:G:460:HIS:O	1:G:464:LEU:HB2	2.19	0.43
1:H:336:PRO:HG2	1:H:337:TYR:HD1	1.82	0.43
1:H:351:LEU:HD21	1:H:357:PRO:HA	2.00	0.43
1:B:323:CYS:HB2	1:B:325:PHE:CE2	2.54	0.43
1:G:126:ILE:HG22	1:G:127:ASP:N	2.33	0.43
1:G:383:ASN:O	1:G:387:ILE:HB	2.18	0.43
1:G:167:TRP:O	1:G:169:VAL:HG12	2.18	0.43
1:G:89:HIS:NE2	1:G:334:TYR:O	2.51	0.43
1:H:83:GLU:HA	1:H:86:TRP:HD1	1.82	0.43
1:C:446:GLY:O	1:C:450:SER:HB2	2.19	0.43
1:B:70:LYS:HA	1:B:70:LYS:HD2	1.53	0.43
1:H:47:ALA:HA	2:H:601:FAD:O2'	2.18	0.43
1:E:158:PHE:CD1	1:E:319:PRO:HG3	2.53	0.43
1:F:187:ASN:OD1	1:F:189:LYS:CB	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:THR:CG2	1:B:400:MET:CG	2.96	0.43
1:H:130:LEU:O	1:H:133:ARG:N	2.51	0.43
2:C:601:FAD:H9	2:C:601:FAD:C2'	2.48	0.43
1:B:411:TYR:CD2	1:B:412:HIS:N	2.87	0.43
1:D:411:TYR:CD2	1:D:412:HIS:N	2.86	0.43
1:E:64:VAL:CG1	1:E:65:ILE:N	2.81	0.43
1:E:298:ILE:O	1:E:298:ILE:HG22	2.16	0.43
1:H:234:THR:HB	1:H:236:PHE:CE2	2.53	0.43
1:G:63:HIS:N	1:G:63:HIS:CD2	2.86	0.43
1:H:420:PRO:HB2	1:H:451:TRP:CD1	2.54	0.43
1:E:325:PHE:HA	1:E:374:VAL:HG13	1.99	0.43
1:D:178:TRP:CB	1:D:454:GLU:CG	2.96	0.43
1:E:155:ALA:HA	1:E:159:MET:HB2	2.01	0.43
1:E:159:MET:HE3	3:E:602:GDU:N3	2.33	0.43
1:G:185:ALA:O	1:G:186:PRO:C	2.57	0.43
1:H:92:ILE:O	1:H:314:CYS:HB2	2.18	0.43
1:H:372:LEU:HD21	1:H:391:CYS:HB3	1.99	0.43
1:A:480:THR:HA	1:A:487:VAL:HG11	1.99	0.43
1:C:495:ARG:O	1:C:496:ARG:HD2	2.19	0.43
1:E:370:ILE:HG22	1:E:372:LEU:HD23	2.00	0.43
1:H:85:ASP:HA	1:H:214:ALA:CB	2.48	0.43
1:A:47:ALA:HB1	1:A:222:TRP:NE1	2.32	0.43
1:F:47:ALA:HB1	1:F:222:TRP:HE1	1.83	0.43
1:E:467:GLU:HG2	1:E:495:ARG:HH22	1.83	0.43
1:H:480:THR:HG23	1:H:487:VAL:HG21	2.00	0.43
1:D:142:PHE:CE1	1:D:179:LEU:HD21	2.53	0.43
1:E:147:VAL:CG2	1:E:160:ARG:HH21	2.30	0.43
1:E:332:SER:HB3	1:E:369:SER:H	1.83	0.43
1:G:109:ASN:C	1:G:111:SER:N	2.72	0.43
1:A:467:GLU:HG2	1:A:495:ARG:HH12	1.83	0.43
1:G:244:LYS:HB3	1:G:244:LYS:HE2	1.93	0.43
1:F:376:GLU:HG2	1:F:377:SER:N	2.33	0.43
1:H:341:GLU:CG	1:H:343:SER:H	2.29	0.43
1:F:137:THR:O	1:F:148:ARG:NH1	2.51	0.43
1:B:389:ALA:HA	1:B:392:ILE:CD1	2.49	0.43
1:B:286:LEU:O	1:B:289:GLN:HG3	2.19	0.43
1:F:321:ASP:N	1:F:321:ASP:OD1	2.46	0.43
1:H:77:ASP:N	1:H:77:ASP:OD1	2.49	0.43
1:B:115:LYS:O	1:B:118:GLN:HB2	2.18	0.43
2:B:601:FAD:O4'	2:B:601:FAD:O2'	2.33	0.43
1:G:455:VAL:HG12	1:G:460:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:TRP:HE3	1:E:146:ILE:N	2.17	0.43
1:E:207:ASN:HB3	1:E:315:TRP:CZ2	2.53	0.43
1:H:351:LEU:HD13	1:H:404:THR:O	2.18	0.43
1:E:69:TYR:CD1	1:E:463:MET:HG3	2.54	0.43
1:C:323:CYS:HB2	1:C:325:PHE:CE2	2.53	0.43
1:C:280:ASP:HB3	1:C:283:LEU:HB2	2.00	0.43
1:H:352:ALA:HB2	1:H:405:ASP:HB2	2.00	0.43
1:G:125:MET:HG2	1:G:188:LEU:CD2	2.48	0.43
1:E:126:ILE:O	1:E:130:LEU:HG	2.18	0.43
1:G:163:ASN:O	1:G:167:TRP:HB2	2.18	0.43
1:C:467:GLU:HG2	1:C:495:ARG:HH12	1.84	0.43
1:B:483:TYR:N	1:B:484:PRO:HD3	2.33	0.43
1:E:368:TRP:HZ3	1:E:370:ILE:HD11	1.80	0.43
1:H:11:LEU:HD21	1:H:252:VAL:CG1	2.49	0.43
1:F:328:ALA:HB2	1:F:372:LEU:HB3	2.00	0.43
1:H:16:GLY:O	1:H:20:LEU:HG	2.19	0.43
3:F:602:GDU:C2	3:F:602:GDU:H5'2	2.48	0.43
1:B:142:PHE:CE1	1:B:179:LEU:HD21	2.54	0.43
1:A:346:LEU:HD13	1:A:408:VAL:CG1	2.48	0.43
1:E:326:TYR:C	1:E:326:TYR:CD1	2.92	0.43
1:E:455:VAL:HA	1:E:460:HIS:ND1	2.23	0.43
1:A:315:TRP:C	1:A:316:LEU:HG	2.38	0.43
1:G:100:GLN:HA	1:G:100:GLN:OE1	2.19	0.43
1:C:423:THR:HB	1:C:425:GLU:OE1	2.18	0.43
1:E:359:SER:OG	1:E:361:GLU:CB	2.66	0.43
1:H:384:GLN:O	1:H:387:ILE:HG22	2.19	0.43
1:E:376:GLU:HB2	1:E:382:VAL:HG13	2.01	0.43
1:B:263:LYS:HD2	1:F:504:PHE:CE1	2.53	0.43
1:D:49:THR:HG22	1:D:50:ASP:N	2.34	0.43
1:B:96:ARG:O	1:B:319:PRO:HD2	2.19	0.43
1:D:346:LEU:HD23	1:D:347:PRO:CD	2.48	0.43
1:G:419:TYR:N	1:G:448:PHE:HZ	2.16	0.43
1:G:204:TRP:HB3	1:G:208:ALA:CB	2.47	0.43
1:H:39:SER:HA	1:H:237:GLY:O	2.18	0.43
1:G:11:LEU:HB3	1:G:265:LEU:CD1	2.48	0.43
1:A:335:SER:OG	1:A:336:PRO:HD2	2.19	0.43
1:A:307:PRO:HB2	1:A:309:ARG:HG2	2.01	0.43
1:F:6:ILE:CG2	1:F:7:SER:N	2.82	0.43
1:D:286:LEU:O	1:D:289:GLN:HG3	2.19	0.43
1:H:256:ASP:OD1	1:H:256:ASP:N	2.46	0.43
1:D:346:LEU:HD23	1:D:347:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:O	1:A:118:GLN:HG3	2.19	0.43
1:H:446:GLY:N	1:H:450:SER:N	2.64	0.43
1:E:69:TYR:O	1:E:72:PHE:HB3	2.18	0.43
1:D:91:ARG:HG3	1:D:315:TRP:CZ2	2.54	0.43
1:H:165:LYS:HD3	1:H:318:PHE:O	2.18	0.43
1:E:306:ARG:HA	1:E:307:PRO:HD3	1.69	0.43
1:B:417:HIS:HB3	1:B:448:PHE:CZ	2.54	0.43
1:B:483:TYR:CE1	1:F:486:PHE:HE1	2.37	0.43
1:B:499:ASP:HB3	1:F:473:VAL:O	2.19	0.43
1:F:291:PHE:CE1	1:F:292:TYR:O	2.72	0.43
1:H:168:ALA:HB1	1:H:377:SER:OG	2.18	0.43
1:B:297:VAL:O	1:B:298:ILE:HD13	2.19	0.43
1:B:77:ASP:O	1:B:81:PRO:HA	2.19	0.43
1:G:443:TRP:HE3	1:G:443:TRP:N	2.17	0.43
1:G:455:VAL:HB	1:G:460:HIS:HB3	2.01	0.43
1:H:270:ALA:HA	1:H:448:PHE:C	2.39	0.43
1:F:9:ASP:HB2	1:F:33:SER:O	2.18	0.43
1:H:479:LEU:HA	1:H:483:TYR:CD2	2.54	0.43
1:E:419:TYR:CE1	2:E:601:FAD:HM73	2.46	0.43
1:F:179:LEU:N	1:F:179:LEU:CD2	2.80	0.43
1:C:350:GLN:NE2	1:C:351:LEU:O	2.52	0.43
1:F:322:ASN:HD21	1:F:398:THR:HG22	1.84	0.43
1:E:94:TYR:CE1	1:E:103:PRO:HG3	2.54	0.43
1:E:12:VAL:CB	1:E:36:ILE:HG13	2.46	0.43
1:G:252:VAL:O	1:G:252:VAL:CG1	2.67	0.43
1:F:506:LYS:HD3	1:F:506:LYS:H	1.84	0.43
1:F:387:ILE:HG23	1:F:388:LEU:H	1.83	0.43
1:G:152:THR:O	1:G:156:ASP:CG	2.56	0.43
1:F:58:TYR:CE1	1:F:299:GLY:HA3	2.54	0.43
1:H:272:ASP:O	1:H:276:GLU:OE2	2.37	0.42
1:B:175:GLN:HE21	1:B:178:TRP:HD1	1.67	0.42
1:G:57:LEU:N	1:G:57:LEU:CD1	2.82	0.42
1:C:125:MET:HG2	1:C:188:LEU:HD13	2.01	0.42
1:H:165:LYS:NZ	1:H:325:PHE:O	2.43	0.42
1:G:387:ILE:HG23	1:G:388:LEU:N	2.34	0.42
1:C:166:VAL:HG13	1:C:167:TRP:CD1	2.53	0.42
1:C:411:TYR:CD2	1:C:412:HIS:N	2.86	0.42
1:C:245:VAL:HG22	1:C:252:VAL:CG2	2.48	0.42
1:E:134:VAL:O	1:E:134:VAL:HG13	2.19	0.42
1:F:291:PHE:CG	1:F:292:TYR:N	2.87	0.42
1:E:436:LYS:O	1:E:439:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HE3	1:A:138:LYS:HB2	1.89	0.42
1:G:272:ASP:O	1:G:275:ALA:N	2.52	0.42
1:G:69:TYR:CG	1:G:463:MET:HG3	2.53	0.42
1:G:309:ARG:HG2	1:G:310:ILE:HD12	2.01	0.42
1:E:318:PHE:CE1	1:E:325:PHE:HE1	2.37	0.42
1:F:122:ILE:HD12	1:F:122:ILE:HA	1.87	0.42
1:H:443:TRP:HB3	1:H:445:ARG:NE	2.33	0.42
1:H:302:VAL:HA	1:H:406:GLU:O	2.18	0.42
1:G:296:HIS:ND1	1:G:412:HIS:HE1	2.17	0.42
1:F:430:LEU:HD23	1:F:430:LEU:HA	1.82	0.42
1:D:13:ILE:HG12	1:D:242:VAL:HG21	2.00	0.42
1:A:204:TRP:CD2	1:A:205:GLY:N	2.85	0.42
1:F:108:ASN:O	1:F:194:ASN:HB3	2.19	0.42
1:H:158:PHE:HE1	1:H:162:TYR:CD2	2.37	0.42
1:H:394:GLY:HA2	1:H:397:ASN:ND2	2.34	0.42
1:H:385:GLU:H	1:H:385:GLU:CD	2.23	0.42
1:C:199:LYS:HD2	1:C:200:THR:N	2.34	0.42
1:E:250:LYS:HA	1:E:262:TYR:CZ	2.55	0.42
1:D:501:ALA:HB2	1:H:473:VAL:HG13	2.01	0.42
1:F:24:LYS:HA	1:F:24:LYS:HD3	1.82	0.42
1:G:77:ASP:OD1	1:G:77:ASP:N	2.49	0.42
1:F:167:TRP:CG	1:F:174:MET:CE	3.02	0.42
1:H:477:VAL:CG2	1:H:478:GLU:N	2.82	0.42
1:E:68:HIS:ND1	1:E:68:HIS:N	2.67	0.42
1:G:471:ASN:HA	1:G:476:ALA:N	2.32	0.42
1:H:402:LYS:H	1:H:402:LYS:HD3	1.84	0.42
1:G:387:ILE:HA	1:G:387:ILE:HD12	1.72	0.42
1:C:47:ALA:CB	1:C:222:TRP:NE1	2.81	0.42
1:E:113:LEU:HB3	1:E:114:PRO:HD2	2.00	0.42
1:G:162:TYR:CE2	1:G:166:VAL:HG11	2.54	0.42
1:C:16:GLY:HA3	2:C:601:FAD:O1P	2.20	0.42
1:F:455:VAL:HG11	1:F:480:THR:O	2.19	0.42
1:C:160:ARG:HB2	1:C:161:PRO:HD3	2.02	0.42
1:D:134:VAL:HG13	1:D:134:VAL:O	2.19	0.42
1:E:467:GLU:HG2	1:E:495:ARG:HH12	1.83	0.42
1:E:445:ARG:NE	1:E:481:LEU:HD22	2.34	0.42
1:G:443:TRP:N	1:G:443:TRP:CE3	2.88	0.42
1:G:309:ARG:HG2	1:G:310:ILE:CD1	2.49	0.42
1:C:107:GLN:H	1:C:107:GLN:CD	2.17	0.42
2:E:601:FAD:O5B	2:E:601:FAD:O1P	2.38	0.42
1:A:60:VAL:O	1:A:63:HIS:CD2	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:302:VAL:HG12	1:H:368:TRP:O	2.20	0.42
1:G:471:ASN:HB2	1:G:476:ALA:O	2.19	0.42
1:H:156:ASP:HA	1:H:160:ARG:HE	1.84	0.42
1:B:204:TRP:CD2	1:B:205:GLY:N	2.86	0.42
1:E:122:ILE:CG2	1:E:123:ASP:N	2.81	0.42
1:B:486:PHE:CE1	1:F:483:TYR:CD1	3.04	0.42
1:H:394:GLY:HA2	1:H:397:ASN:HB2	2.01	0.42
1:A:32:PRO:CG	1:E:504:PHE:HD2	2.33	0.42
1:B:386:THR:OG1	1:B:387:ILE:N	2.53	0.42
1:H:89:HIS:NE2	1:H:334:TYR:HA	2.34	0.42
1:H:453:TYR:O	1:H:454:GLU:C	2.57	0.42
1:E:168:ALA:HB1	1:E:380:LYS:HB3	2.00	0.42
1:H:24:LYS:HD3	1:H:24:LYS:HA	1.69	0.42
1:F:422:PRO:HA	1:F:426:ARG:HD3	2.01	0.42
1:F:143:ASP:OD2	1:F:171:THR:OG1	2.34	0.42
1:B:458:GLN:HG3	2:B:601:FAD:N1	2.33	0.42
2:H:601:FAD:H9	2:H:601:FAD:H1'1	1.34	0.42
1:C:175:GLN:HE22	1:C:177:ALA:HB3	1.85	0.42
1:E:16:GLY:H	2:E:601:FAD:H4B	1.84	0.42
1:G:303:ARG:NH2	1:G:346:LEU:O	2.52	0.42
1:F:352:ALA:HB3	1:F:403:PRO:HA	2.01	0.42
1:E:438:GLN:NE2	1:E:442:ILE:O	2.48	0.42
1:H:235:ARG:HE	1:H:235:ARG:HB3	1.51	0.42
1:E:110:ILE:HG13	1:E:113:LEU:HD12	2.02	0.42
1:F:5:ASP:N	1:F:259:THR:OG1	2.30	0.42
1:B:483:TYR:O	1:B:486:PHE:HB3	2.19	0.42
1:B:69:TYR:CD2	1:B:463:MET:HG3	2.54	0.42
1:C:38:ASP:HA	2:C:601:FAD:C2A	2.48	0.42
1:F:345:LYS:HG2	1:F:364:GLU:HG3	2.01	0.42
1:E:129:ALA:O	1:E:132:ALA:HB3	2.20	0.42
1:E:396:VAL:HA	1:E:401:LEU:HB2	2.01	0.42
1:E:70:LYS:CB	1:E:496:ARG:HH12	2.29	0.42
1:D:332:SER:OG	1:D:369:SER:N	2.42	0.42
1:H:447:ARG:HG2	1:H:448:PHE:CE2	2.54	0.42
1:A:174:MET:HB2	1:A:422:PRO:O	2.18	0.42
1:A:175:GLN:HG3	1:A:422:PRO:O	2.19	0.42
1:D:280:ASP:HB3	1:D:283:LEU:HB2	2.02	0.42
1:G:102:VAL:CG1	1:G:109:ASN:HB3	2.50	0.42
1:C:291:PHE:O	1:C:421:THR:HB	2.20	0.42
1:E:303:ARG:HH22	1:E:363:LYS:HG3	1.79	0.42
1:E:437:LEU:O	1:E:442:ILE:N	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:GLU:O	1:E:428:GLY:C	2.58	0.42
1:G:11:LEU:HB3	1:G:265:LEU:HD12	2.01	0.42
1:C:331:PHE:HD1	1:C:331:PHE:HA	1.73	0.42
1:E:205:GLY:HA2	1:E:206:PRO:HD3	1.74	0.42
1:A:443:TRP:CD1	1:A:445:ARG:NH2	2.88	0.42
1:G:367:TYR:CD1	1:G:408:VAL:HG21	2.51	0.42
1:B:57:LEU:HD22	1:B:338:ASN:HA	2.02	0.42
1:D:244:LYS:HG2	1:D:245:VAL:H	1.84	0.42
1:A:57:LEU:N	1:A:57:LEU:HD12	2.35	0.42
1:G:402:LYS:HB2	1:G:402:LYS:HE2	1.68	0.42
1:D:182:ARG:HD2	3:D:602:GDU:O2A	2.19	0.42
1:G:85:ASP:HA	1:G:214:ALA:HB2	2.02	0.42
1:E:231:LYS:HB3	1:E:231:LYS:HE2	1.71	0.42
3:F:602:GDU:H6	3:F:602:GDU:H2D	1.85	0.42
1:B:150:MET:HG2	1:B:154:ILE:HG21	2.02	0.42
1:H:483:TYR:CD2	1:H:483:TYR:N	2.87	0.42
1:E:146:ILE:H	1:E:146:ILE:HG13	1.72	0.42
1:E:159:MET:HE1	3:E:602:GDU:C2	2.49	0.42
1:D:38:ASP:HA	2:D:601:FAD:C2A	2.50	0.42
1:D:63:HIS:CD2	2:D:601:FAD:C6	3.03	0.42
1:G:92:ILE:HG22	1:G:94:TYR:HE2	1.84	0.42
1:G:102:VAL:HA	1:G:103:PRO:HD3	1.78	0.42
1:G:70:LYS:HE2	1:G:496:ARG:NH1	2.35	0.42
1:H:25:ARG:NH2	1:H:495:ARG:HG3	2.34	0.42
1:H:71:TYR:CD2	1:H:496:ARG:C	2.93	0.42
1:D:158:PHE:CZ	3:D:602:GDU:N3	2.87	0.42
1:D:473:VAL:HG12	1:H:501:ALA:CA	2.50	0.42
1:G:27:ASN:O	1:G:30:ASP:HB2	2.20	0.42
1:D:443:TRP:CE3	1:D:443:TRP:N	2.88	0.42
1:B:100:GLN:OE1	1:B:100:GLN:HA	2.19	0.42
1:F:26:LEU:HD22	1:F:34:TRP:HB3	2.02	0.42
1:A:447:ARG:HB2	2:A:601:FAD:H5'2	2.02	0.42
1:H:156:ASP:HB2	1:H:157:LEU:HD12	2.02	0.42
1:B:331:PHE:HB3	1:B:369:SER:HB3	2.01	0.42
1:C:296:HIS:NE2	1:C:382:VAL:HG21	2.34	0.42
1:C:499:ASP:HB3	1:G:473:VAL:O	2.19	0.42
1:C:306:ARG:HA	1:C:307:PRO:HD3	1.82	0.42
1:B:35:MET:HE1	1:B:235:ARG:HG3	2.00	0.42
1:D:27:ASN:HD22	1:D:27:ASN:C	2.23	0.42
1:G:425:GLU:CD	1:G:425:GLU:H	2.22	0.42
1:D:8:VAL:HG11	1:D:35:MET:HG2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:THR:HG22	1:E:50:ASP:N	2.35	0.42
1:A:407:ILE:HG22	1:A:407:ILE:O	2.19	0.42
1:H:30:ASP:O	1:H:30:ASP:OD1	2.37	0.42
1:G:47:ALA:HA	1:G:63:HIS:HE1	1.83	0.42
1:D:178:TRP:CH2	1:D:179:LEU:HD23	2.55	0.42
1:D:423:THR:O	1:D:426:ARG:HB2	2.19	0.42
1:G:388:LEU:O	1:G:392:ILE:HG13	2.20	0.42
1:C:433:ILE:O	1:C:436:LYS:HB2	2.20	0.42
1:G:258:THR:CG2	1:G:259:THR:N	2.82	0.42
1:F:413:ARG:HG2	1:F:414:ARG:N	2.35	0.42
1:F:7:SER:HA	1:F:261:GLY:O	2.20	0.42
1:C:483:TYR:O	1:C:486:PHE:HB3	2.19	0.42
1:G:110:ILE:HG13	1:G:113:LEU:HD12	2.01	0.42
1:B:106:PHE:HD2	1:B:106:PHE:C	2.23	0.42
1:C:287:THR:O	1:C:290:LEU:HD12	2.20	0.42
1:B:158:PHE:CE2	1:B:159:MET:HE1	2.55	0.42
1:B:317:TYR:HE1	3:B:602:GDU:O1B	2.03	0.42
1:C:494:GLU:OE1	1:C:494:GLU:N	2.46	0.42
1:H:302:VAL:HG13	1:H:368:TRP:CG	2.55	0.42
1:G:302:VAL:HG13	1:G:368:TRP:CG	2.55	0.42
1:B:111:SER:HB2	1:B:112:MET:HE3	2.02	0.42
1:H:401:LEU:HA	1:H:405:ASP:OD2	2.20	0.42
1:H:402:LYS:HE2	1:H:402:LYS:HB2	1.63	0.42
1:G:387:ILE:HA	1:G:390:ASP:OD2	2.19	0.42
1:H:82:LYS:HE2	1:H:84:ASP:OD1	2.19	0.42
1:H:297:VAL:HB	1:H:415:PHE:CE2	2.47	0.42
1:F:168:ALA:HB1	1:F:377:SER:OG	2.20	0.42
1:A:411:TYR:CD2	1:A:412:HIS:N	2.87	0.42
1:D:199:LYS:HD2	1:D:200:THR:N	2.35	0.42
1:B:437:LEU:HD12	1:B:444:SER:HB2	2.00	0.42
1:C:446:GLY:H	1:C:450:SER:HB2	1.85	0.42
1:F:46:LEU:O	1:F:60:VAL:HG21	2.20	0.42
1:E:467:GLU:CG	1:E:495:ARG:NH1	2.83	0.41
1:F:158:PHE:C	1:F:158:PHE:CD1	2.92	0.41
1:G:104:TYR:CG	1:G:105:PRO:HA	2.55	0.41
3:E:602:GDU:O5'	3:E:602:GDU:O1B	2.37	0.41
1:A:139:PRO:HB2	1:A:176:CYS:SG	2.60	0.41
1:G:307:PRO:HG2	1:G:368:TRP:CZ2	2.55	0.41
1:G:335:SER:HB3	1:G:338:ASN:OD1	2.19	0.41
1:F:94:TYR:CE1	1:F:103:PRO:HG3	2.55	0.41
1:H:235:ARG:O	1:H:240:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:271:VAL:HG13	1:E:287:THR:CG2	2.49	0.41
1:G:210:PHE:H	1:G:210:PHE:HD2	1.66	0.41
1:A:250:LYS:HA	1:A:262:TYR:CZ	2.55	0.41
1:G:61:GLY:HA2	1:G:373:GLU:OE1	2.20	0.41
1:B:477:VAL:CG2	1:B:478:GLU:N	2.83	0.41
1:F:16:GLY:O	1:F:19:GLY:N	2.53	0.41
1:E:469:VAL:O	1:E:472:ILE:N	2.54	0.41
1:E:145:TRP:HH2	1:E:183:VAL:HG21	1.81	0.41
1:A:175:GLN:HG3	1:A:175:GLN:H	1.55	0.41
1:H:471:ASN:HB2	1:H:476:ALA:O	2.20	0.41
1:G:90:GLN:O	1:G:92:ILE:HG12	2.20	0.41
1:D:110:ILE:CA	1:D:113:LEU:HD12	2.43	0.41
1:G:130:LEU:O	1:G:133:ARG:CB	2.64	0.41
1:G:167:TRP:CZ2	1:G:178:TRP:CH2	3.08	0.41
1:B:484:PRO:HA	1:B:487:VAL:HG22	2.02	0.41
1:H:71:TYR:HB2	1:H:495:ARG:O	2.20	0.41
1:H:499:ASP:O	1:H:500:GLY:C	2.58	0.41
1:A:268:THR:HA	1:A:445:ARG:O	2.20	0.41
1:D:57:LEU:N	1:D:57:LEU:HD12	2.35	0.41
1:F:42:THR:HA	1:F:43:PRO:HD2	1.85	0.41
1:H:122:ILE:HA	1:H:122:ILE:HD13	1.96	0.41
1:E:221:ILE:H	1:E:221:ILE:HG13	1.66	0.41
1:E:510:GLN:N	1:E:510:GLN:OE1	2.53	0.41
1:F:153:GLY:O	1:F:157:LEU:HB2	2.20	0.41
1:B:447:ARG:HB2	2:B:601:FAD:H5'2	2.00	0.41
1:B:16:GLY:CA	2:B:601:FAD:O1A	2.67	0.41
1:C:339:GLN:N	1:C:339:GLN:CD	2.74	0.41
1:H:124:GLY:HA3	1:H:153:GLY:H	1.86	0.41
1:F:263:LYS:N	1:F:263:LYS:HD2	2.36	0.41
1:F:122:ILE:O	1:F:125:MET:N	2.53	0.41
1:C:115:LYS:O	1:C:118:GLN:HB2	2.19	0.41
1:E:183:VAL:CG1	3:E:602:GDU:C2	2.99	0.41
1:A:176:CYS:HA	1:A:179:LEU:HD11	2.01	0.41
1:H:107:GLN:O	1:H:110:ILE:HG22	2.21	0.41
1:E:125:MET:CG	1:E:188:LEU:HD13	2.48	0.41
1:G:499:ASP:O	1:G:500:GLY:C	2.57	0.41
1:G:166:VAL:HG12	1:G:326:TYR:CB	2.50	0.41
1:C:146:ILE:HG23	1:C:150:MET:HE3	2.02	0.41
1:H:499:ASP:O	1:H:502:GLN:N	2.52	0.41
1:A:389:ALA:HA	1:A:392:ILE:CD1	2.50	0.41
1:G:453:TYR:O	1:G:454:GLU:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:LYS:O	1:A:254:LEU:HD13	2.20	0.41
1:D:150:MET:HG2	1:D:154:ILE:CG2	2.49	0.41
1:B:94:TYR:H	1:B:316:LEU:HB3	1.85	0.41
1:A:304:GLY:O	1:A:368:TRP:HD1	2.04	0.41
1:E:213:PRO:HG2	1:E:217:GLY:O	2.21	0.41
1:A:8:VAL:HA	1:A:33:SER:OG	2.19	0.41
1:E:417:HIS:HB3	1:E:448:PHE:CZ	2.54	0.41
1:F:231:LYS:HE2	1:F:231:LYS:HB3	1.73	0.41
1:H:164:PHE:CD1	1:H:164:PHE:C	2.92	0.41
1:F:142:PHE:HB3	1:F:174:MET:HB2	2.02	0.41
1:E:18:THR:HG23	1:E:461:SER:O	2.20	0.41
1:G:18:THR:HG22	1:G:19:GLY:N	2.34	0.41
1:C:303:ARG:NH2	1:C:363:LYS:C	2.68	0.41
1:D:325:PHE:CA	1:D:374:VAL:HG22	2.50	0.41
1:H:383:ASN:OD1	1:H:385:GLU:HG2	2.21	0.41
1:G:329:THR:HG21	1:G:334:TYR:CE2	2.56	0.41
3:D:602:GDU:O1B	3:D:602:GDU:H3'	2.19	0.41
1:C:199:LYS:HB3	1:C:199:LYS:HE2	1.69	0.41
1:B:443:TRP:HD1	1:B:445:ARG:HH21	1.66	0.41
1:C:304:GLY:O	1:C:368:TRP:CD1	2.74	0.41
1:B:133:ARG:NH2	1:H:134:VAL:HG21	2.35	0.41
1:G:175:GLN:HG2	1:G:422:PRO:O	2.21	0.41
1:B:446:GLY:H	1:B:450:SER:HB2	1.84	0.41
1:B:299:GLY:HA2	1:B:370:ILE:O	2.20	0.41
1:F:68:HIS:N	1:F:68:HIS:ND1	2.67	0.41
1:D:299:GLY:HA2	1:D:370:ILE:O	2.20	0.41
1:E:91:ARG:HB2	1:E:207:ASN:O	2.21	0.41
1:G:337:TYR:N	1:G:337:TYR:HD1	2.17	0.41
1:F:207:ASN:HB3	1:F:315:TRP:HH2	1.83	0.41
1:G:387:ILE:CG2	1:G:388:LEU:N	2.83	0.41
1:E:294:SER:CB	1:E:414:ARG:NH2	2.83	0.41
1:B:199:LYS:HB3	1:B:199:LYS:HE2	1.71	0.41
1:E:43:PRO:HG2	1:E:223:ILE:HD13	2.02	0.41
1:E:447:ARG:O	1:E:451:TRP:HA	2.20	0.41
1:H:116:GLU:OE2	1:H:117:GLU:HG2	2.21	0.41
1:H:120:LYS:HE3	1:H:120:LYS:HB2	1.82	0.41
1:F:183:VAL:HG12	3:F:602:GDU:C2	2.50	0.41
1:E:468:ALA:O	1:E:472:ILE:HG13	2.20	0.41
1:D:331:PHE:HD1	1:D:331:PHE:HA	1.72	0.41
1:F:122:ILE:CG2	1:F:126:ILE:HD11	2.47	0.41
1:H:308:GLU:HG3	1:H:309:ARG:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:139:PRO:HA	1:H:144:GLU:OE2	2.21	0.41
1:G:25:ARG:HA	1:G:28:GLN:CB	2.50	0.41
1:G:28:GLN:CG	1:G:497:LEU:HD12	2.50	0.41
1:D:166:VAL:HG13	1:D:167:TRP:CD1	2.55	0.41
1:F:270:ALA:HB3	1:F:273:PHE:HD2	1.83	0.41
1:F:397:ASN:C	1:F:399:GLU:N	2.74	0.41
1:G:120:LYS:HE3	1:G:120:LYS:HB2	1.76	0.41
1:D:106:PHE:CD2	1:D:106:PHE:C	2.94	0.41
1:F:104:TYR:CG	1:F:105:PRO:HA	2.55	0.41
1:D:331:PHE:HB3	1:D:369:SER:HB3	2.03	0.41
1:E:142:PHE:CB	1:E:174:MET:HB2	2.50	0.41
1:E:457:ASN:C	2:E:601:FAD:O3'	2.59	0.41
1:F:178:TRP:CD2	1:F:179:LEU:HD22	2.55	0.41
1:B:398:THR:O	1:B:399:GLU:HB2	2.21	0.41
1:H:92:ILE:HG22	1:H:94:TYR:HE2	1.85	0.41
1:A:69:TYR:CD1	1:A:463:MET:HG3	2.55	0.41
1:G:160:ARG:N	1:G:161:PRO:HD2	2.36	0.41
1:C:63:HIS:CD2	2:C:601:FAD:C6	3.04	0.41
1:F:364:GLU:HA	1:F:367:TYR:OH	2.20	0.41
1:B:244:LYS:HG2	1:B:245:VAL:H	1.85	0.41
1:C:503:VAL:HA	1:C:506:LYS:HE2	2.03	0.41
1:A:6:ILE:O	1:A:260:ILE:HA	2.20	0.41
1:D:469:VAL:O	1:D:472:ILE:N	2.54	0.41
1:E:139:PRO:HA	1:E:144:GLU:CD	2.41	0.41
1:H:80:LEU:HA	1:H:81:PRO:HD2	1.89	0.41
1:D:58:TYR:HE1	1:D:369:SER:HG	1.66	0.41
1:D:176:CYS:HA	1:D:179:LEU:HD11	2.02	0.41
1:B:175:GLN:HG3	1:B:175:GLN:H	1.60	0.41
1:E:38:ASP:OD1	2:E:601:FAD:H1B	2.20	0.41
1:E:150:MET:HG3	1:E:154:ILE:HB	2.02	0.41
1:F:187:ASN:CG	1:F:189:LYS:HB2	2.39	0.41
1:A:420:PRO:O	1:A:422:PRO:HD3	2.20	0.41
1:D:458:GLN:CA	2:D:601:FAD:O3'	2.68	0.41
1:C:150:MET:HG2	1:C:154:ILE:HG21	2.02	0.41
1:F:306:ARG:HG2	1:F:306:ARG:O	2.19	0.41
1:A:329:THR:O	1:A:370:ILE:HA	2.21	0.41
1:G:80:LEU:HA	1:G:81:PRO:HD2	1.90	0.41
1:D:5:ASP:OD2	1:D:258:THR:HA	2.21	0.41
1:E:152:THR:O	1:E:153:GLY:C	2.57	0.41
1:E:497:LEU:HA	1:E:497:LEU:HD12	1.92	0.41
1:F:26:LEU:HD13	1:F:34:TRP:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:THR:HA	1:E:462:PHE:HA	2.02	0.41
1:B:339:GLN:OE1	1:B:339:GLN:N	2.54	0.41
1:B:110:ILE:CG2	1:B:118:GLN:HG2	2.51	0.41
1:H:273:PHE:CZ	1:H:417:HIS:NE2	2.89	0.41
1:H:480:THR:CA	1:H:487:VAL:HG11	2.51	0.41
1:B:420:PRO:O	1:B:422:PRO:HD3	2.21	0.41
1:H:298:ILE:HG23	1:H:411:TYR:O	2.20	0.41
1:E:178:TRP:CD2	1:E:179:LEU:HD22	2.56	0.41
1:B:204:TRP:CE3	1:B:205:GLY:N	2.88	0.41
1:G:103:PRO:HD2	1:G:109:ASN:CG	2.41	0.41
1:G:383:ASN:OD1	1:G:385:GLU:HG2	2.21	0.41
1:C:145:TRP:HB2	1:C:176:CYS:CB	2.51	0.41
1:C:142:PHE:CE1	1:C:179:LEU:HD21	2.56	0.41
1:G:252:VAL:HG13	1:G:254:LEU:CD2	2.51	0.41
1:H:28:GLN:CG	1:H:497:LEU:HD12	2.51	0.41
1:C:223:ILE:HA	1:C:223:ILE:HD13	1.92	0.41
1:F:350:GLN:HE22	1:F:407:ILE:HD12	1.84	0.41
1:A:134:VAL:O	1:A:134:VAL:HG13	2.21	0.41
1:B:8:VAL:O	1:B:262:TYR:HA	2.21	0.41
1:F:392:ILE:O	1:F:395:LEU:HB2	2.21	0.41
1:D:389:ALA:HA	1:D:392:ILE:CD1	2.51	0.41
1:C:35:MET:HE2	1:C:35:MET:HB2	1.88	0.41
1:C:389:ALA:HA	1:C:392:ILE:CD1	2.50	0.41
1:F:328:ALA:CB	1:F:372:LEU:HB3	2.51	0.41
1:A:278:MET:O	1:A:279:ASN:HB2	2.20	0.41
1:A:12:VAL:HB	1:A:36:ILE:HB	2.02	0.41
1:B:328:ALA:HB2	1:B:372:LEU:HB3	2.02	0.41
1:D:376:GLU:HA	1:D:380:LYS:O	2.21	0.41
1:H:34:TRP:HH2	1:H:229:LEU:HD22	1.85	0.41
1:E:108:ASN:O	1:E:194:ASN:HB3	2.21	0.41
1:A:286:LEU:O	1:A:289:GLN:HG3	2.20	0.41
1:G:313:LYS:H	1:G:313:LYS:HG3	1.71	0.41
1:G:136:ASN:N	1:G:136:ASN:OD1	2.47	0.41
1:C:256:ASP:N	1:C:256:ASP:OD2	2.51	0.41
1:F:146:ILE:H	1:F:146:ILE:HG13	1.72	0.41
1:C:56:PHE:CE1	1:C:339:GLN:HB3	2.56	0.41
1:H:128:ALA:HB2	1:H:151:GLY:HA2	2.02	0.41
1:D:494:GLU:OE2	1:H:477:VAL:HB	2.21	0.41
1:H:351:LEU:HB2	1:H:355:SER:H	1.87	0.41
1:A:91:ARG:HG3	1:A:315:TRP:CZ2	2.55	0.41
1:B:423:THR:HB	1:B:425:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ARG:HG2	1:E:414:ARG:H	1.85	0.41
1:D:42:THR:HA	1:D:43:PRO:HD2	1.82	0.41
1:E:506:LYS:H	1:E:506:LYS:HD3	1.85	0.41
1:B:250:LYS:HA	1:B:262:TYR:CZ	2.56	0.41
1:H:83:GLU:HA	1:H:86:TRP:CD1	2.55	0.41
1:H:66:PHE:CD1	1:H:67:SER:N	2.89	0.41
1:A:376:GLU:HA	1:A:380:LYS:O	2.20	0.41
1:E:18:THR:HG23	1:E:464:LEU:HB2	2.01	0.40
1:B:56:PHE:CE1	1:B:339:GLN:HB3	2.56	0.40
1:B:62:GLY:O	3:B:602:GDU:C6'	2.69	0.40
1:G:115:LYS:HA	1:G:118:GLN:CG	2.35	0.40
1:H:351:LEU:CD1	1:H:404:THR:HA	2.50	0.40
1:G:307:PRO:HG2	1:G:368:TRP:CH2	2.57	0.40
1:G:57:LEU:HD11	1:G:337:TYR:O	2.21	0.40
1:D:63:HIS:HB3	1:D:458:GLN:HE22	1.86	0.40
1:E:192:THR:O	1:E:193:THR:C	2.59	0.40
1:H:160:ARG:HB2	1:H:161:PRO:CD	2.51	0.40
1:F:80:LEU:HA	1:F:81:PRO:HD2	1.90	0.40
1:B:60:VAL:O	1:B:63:HIS:CD2	2.75	0.40
1:H:90:GLN:HA	1:H:209:THR:HG23	2.03	0.40
1:F:145:TRP:HE3	1:F:146:ILE:N	2.20	0.40
1:F:143:ASP:N	1:F:171:THR:O	2.53	0.40
1:G:271:VAL:HG13	1:G:272:ASP:H	1.86	0.40
1:H:63:HIS:HA	2:H:601:FAD:C4	2.51	0.40
1:C:110:ILE:O	1:C:113:LEU:HB2	2.20	0.40
1:E:104:TYR:CE1	3:E:602:GDU:O4	2.75	0.40
1:A:60:VAL:HB	1:A:63:HIS:CE1	2.56	0.40
1:A:175:GLN:HE21	1:A:178:TRP:HD1	1.69	0.40
1:G:336:PRO:HG2	1:G:337:TYR:HD1	1.83	0.40
1:B:194:ASN:HA	1:B:194:ASN:HD22	1.56	0.40
1:G:235:ARG:O	1:G:240:GLY:HA3	2.21	0.40
1:F:414:ARG:HG2	1:F:415:PHE:N	2.36	0.40
1:A:306:ARG:HA	1:A:307:PRO:HD3	1.81	0.40
1:G:9:ASP:HA	1:G:263:LYS:HD3	2.03	0.40
1:C:250:LYS:HA	1:C:262:TYR:CZ	2.56	0.40
1:D:278:MET:CE	1:D:442:ILE:HD12	2.51	0.40
1:E:77:ASP:OD1	1:E:211:ARG:NH1	2.53	0.40
1:H:239:LYS:HE3	1:H:239:LYS:HB2	1.91	0.40
1:G:270:ALA:HA	1:G:448:PHE:O	2.21	0.40
1:G:196:ILE:HG22	1:G:197:LEU:HD23	2.03	0.40
1:H:222:TRP:O	1:H:226:ALA:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:SER:OG	1:E:274:LEU:HD22	2.21	0.40
1:G:235:ARG:O	1:G:236:PHE:CD1	2.74	0.40
1:E:348:THR:HG23	1:E:407:ILE:N	2.36	0.40
1:G:497:LEU:HD12	1:G:497:LEU:O	2.21	0.40
1:C:128:ALA:HB1	1:C:148:ARG:O	2.21	0.40
1:C:469:VAL:O	1:C:473:VAL:HG23	2.21	0.40
1:D:306:ARG:HA	1:D:307:PRO:HD3	1.83	0.40
1:F:139:PRO:HA	1:F:144:GLU:CD	2.42	0.40
1:A:296:HIS:NE2	1:A:382:VAL:HG21	2.36	0.40
1:G:237:GLY:C	1:G:239:LYS:N	2.73	0.40
1:B:146:ILE:HG23	1:B:150:MET:HE3	2.03	0.40
1:G:464:LEU:HD21	1:G:481:LEU:N	2.36	0.40
1:E:63:HIS:HB2	1:E:458:GLN:HE22	1.86	0.40
1:E:69:TYR:HB2	1:E:72:PHE:CB	2.52	0.40
1:B:91:ARG:O	1:B:92:ILE:HD13	2.21	0.40
1:F:91:ARG:HG3	1:F:315:TRP:CZ2	2.55	0.40
1:D:495:ARG:O	1:D:496:ARG:HD2	2.22	0.40
1:C:443:TRP:CE3	1:C:443:TRP:N	2.89	0.40
1:H:70:LYS:HG3	1:H:496:ARG:NH1	2.36	0.40
1:A:108:ASN:HB2	1:A:194:ASN:OD1	2.21	0.40
1:H:283:LEU:HD13	1:H:437:LEU:HD21	2.03	0.40
1:D:335:SER:HB3	1:D:338:ASN:OD1	2.21	0.40
1:H:384:GLN:HG2	1:H:384:GLN:H	1.56	0.40
1:B:433:ILE:HG22	1:B:434:LEU:N	2.36	0.40
1:B:166:VAL:HG13	1:B:167:TRP:CD1	2.56	0.40
1:D:249:ASN:O	1:D:251:THR:HG23	2.22	0.40
1:H:95:VAL:HG22	1:H:317:TYR:CD2	2.55	0.40
1:A:242:VAL:HA	1:A:254:LEU:HD22	2.03	0.40
1:D:94:TYR:H	1:D:316:LEU:HB3	1.85	0.40
1:G:421:THR:HA	1:G:422:PRO:HD3	1.71	0.40
1:F:347:PRO:HA	1:F:361:GLU:O	2.21	0.40
1:F:66:PHE:HB3	1:F:206:PRO:O	2.21	0.40
1:F:40:ASN:O	1:F:236:PHE:HB3	2.22	0.40
1:F:65:ILE:O	1:F:210:PHE:HB3	2.21	0.40
1:D:46:LEU:HB2	2:D:601:FAD:O4'	2.22	0.40
1:E:307:PRO:CB	1:E:309:ARG:HE	2.35	0.40
1:C:443:TRP:CD1	1:C:445:ARG:NH2	2.90	0.40
1:C:268:THR:HA	1:C:445:ARG:O	2.21	0.40
1:F:204:TRP:CE3	1:F:205:GLY:CA	3.05	0.40
1:C:335:SER:OG	1:C:336:PRO:HD2	2.22	0.40
1:E:65:ILE:O	1:E:210:PHE:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:388:LEU:HD13	1:F:388:LEU:HA	1.97	0.40
1:E:82:LYS:HB2	1:E:85:ASP:CG	2.42	0.40
1:H:65:ILE:O	1:H:65:ILE:CG2	2.68	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	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	52	84
1	B	507/509 (100%)	476 (94%)	29 (6%)	2 (0%)	39	75
1	C	507/509 (100%)	476 (94%)	30 (6%)	1 (0%)	52	84
1	D	507/509 (100%)	481 (95%)	25 (5%)	1 (0%)	52	84
1	E	507/509 (100%)	456 (90%)	51 (10%)	0	100	100
1	F	507/509 (100%)	457 (90%)	49 (10%)	1 (0%)	52	84
1	G	507/509 (100%)	462 (91%)	45 (9%)	0	100	100
1	H	507/509 (100%)	460 (91%)	46 (9%)	1 (0%)	52	84
All	All	4056/4072 (100%)	3744 (92%)	305 (8%)	7 (0%)	52	84

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	203	ASN
1	B	61	GLY
1	A	107	GLN
1	B	107	GLN
1	C	107	GLN
1	D	107	GLN
1	F	60	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	430/430 (100%)	372 (86%)	58 (14%)	5	20
1	B	430/430 (100%)	367 (85%)	63 (15%)	4	16
1	C	430/430 (100%)	370 (86%)	60 (14%)	4	18
1	D	430/430 (100%)	366 (85%)	64 (15%)	4	15
1	E	430/430 (100%)	363 (84%)	67 (16%)	3	14
1	F	430/430 (100%)	359 (84%)	71 (16%)	3	12
1	G	430/430 (100%)	347 (81%)	83 (19%)	2	8
1	H	430/430 (100%)	351 (82%)	79 (18%)	2	9
All	All	3440/3440 (100%)	2895 (84%)	545 (16%)	3	13

All (545) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ILE
1	A	35	MET
1	A	40	ASN
1	A	57	LEU
1	A	65	ILE
1	A	67	SER
1	A	82	LYS
1	A	88	THR
1	A	89	HIS
1	A	95	VAL
1	A	106	PHE
1	A	108	ASN
1	A	111	SER
1	A	112	MET
1	A	122	ILE
1	A	140	LYS
1	A	149	MET
1	A	150	MET
1	A	152	THR

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Mol	Chain	Res	Type
1	A	175	GLN
1	A	179	LEU
1	A	199	LYS
1	A	209	THR
1	A	232	GLU
1	A	241	LYS
1	A	252	VAL
1	A	271	VAL
1	A	274	LEU
1	A	281	GLN
1	A	286	LEU
1	A	293	SER
1	A	316	LEU
1	A	317	TYR
1	A	331	PHE
1	A	332	SER
1	A	338	ASN
1	A	339	GLN
1	A	350	GLN
1	A	351	LEU
1	A	358	GLN
1	A	359	SER
1	A	360	THR
1	A	372	LEU
1	A	384	GLN
1	A	392	ILE
1	A	393	GLN
1	A	404	THR
1	A	411	TYR
1	A	424	LEU
1	A	433	ILE
1	A	450	SER
1	A	455	VAL
1	A	473	VAL
1	A	477	VAL
1	A	478	GLU
1	A	485	ASP
1	A	506	LYS
1	A	510	GLN
1	B	6	ILE
1	B	35	MET
1	B	40	ASN

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Mol	Chain	Res	Type
1	B	57	LEU
1	B	65	ILE
1	B	67	SER
1	B	68	HIS
1	B	70	LYS
1	B	82	LYS
1	B	88	THR
1	B	89	HIS
1	B	95	VAL
1	B	106	PHE
1	B	107	GLN
1	B	108	ASN
1	B	111	SER
1	B	112	MET
1	B	116	GLU
1	B	140	LYS
1	B	149	MET
1	B	150	MET
1	B	152	THR
1	B	175	GLN
1	B	179	LEU
1	B	194	ASN
1	B	199	LYS
1	B	209	THR
1	B	232	GLU
1	B	241	LYS
1	B	252	VAL
1	B	274	LEU
1	B	281	GLN
1	B	284	VAL
1	B	286	LEU
1	B	293	SER
1	B	316	LEU
1	B	317	TYR
1	B	331	PHE
1	B	332	SER
1	B	338	ASN
1	B	339	GLN
1	B	350	GLN
1	B	360	THR
1	B	369	SER
1	B	372	LEU

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Mol	Chain	Res	Type
1	B	373	GLU
1	B	384	GLN
1	B	392	ILE
1	B	393	GLN
1	B	404	THR
1	B	411	TYR
1	B	424	LEU
1	B	433	ILE
1	B	444	SER
1	B	450	SER
1	B	451	TRP
1	B	455	VAL
1	B	473	VAL
1	B	477	VAL
1	B	478	GLU
1	B	485	ASP
1	B	506	LYS
1	B	510	GLN
1	C	6	ILE
1	C	35	MET
1	C	40	ASN
1	C	42	THR
1	C	57	LEU
1	C	65	ILE
1	C	67	SER
1	C	68	HIS
1	C	70	LYS
1	C	82	LYS
1	C	88	THR
1	C	89	HIS
1	C	95	VAL
1	C	106	PHE
1	C	107	GLN
1	C	108	ASN
1	C	111	SER
1	C	112	MET
1	C	116	GLU
1	C	140	LYS
1	C	149	MET
1	C	150	MET
1	C	152	THR
1	C	175	GLN

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Mol	Chain	Res	Type
1	C	179	LEU
1	C	199	LYS
1	C	209	THR
1	C	232	GLU
1	C	241	LYS
1	C	252	VAL
1	C	271	VAL
1	C	274	LEU
1	C	281	GLN
1	C	284	VAL
1	C	286	LEU
1	C	293	SER
1	C	316	LEU
1	C	317	TYR
1	C	331	PHE
1	C	332	SER
1	C	338	ASN
1	C	339	GLN
1	C	350	GLN
1	C	351	LEU
1	C	360	THR
1	C	372	LEU
1	C	373	GLU
1	C	384	GLN
1	C	393	GLN
1	C	404	THR
1	C	410	THR
1	C	411	TYR
1	C	424	LEU
1	C	433	ILE
1	C	444	SER
1	C	455	VAL
1	C	473	VAL
1	C	477	VAL
1	C	485	ASP
1	C	510	GLN
1	D	6	ILE
1	D	27	ASN
1	D	35	MET
1	D	40	ASN
1	D	57	LEU
1	D	65	ILE

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Mol	Chain	Res	Type
1	D	67	SER
1	D	70	LYS
1	D	82	LYS
1	D	88	THR
1	D	89	HIS
1	D	95	VAL
1	D	106	PHE
1	D	107	GLN
1	D	108	ASN
1	D	111	SER
1	D	112	MET
1	D	140	LYS
1	D	149	MET
1	D	150	MET
1	D	152	THR
1	D	175	GLN
1	D	179	LEU
1	D	199	LYS
1	D	209	THR
1	D	232	GLU
1	D	241	LYS
1	D	252	VAL
1	D	271	VAL
1	D	274	LEU
1	D	281	GLN
1	D	284	VAL
1	D	286	LEU
1	D	293	SER
1	D	316	LEU
1	D	317	TYR
1	D	331	PHE
1	D	332	SER
1	D	338	ASN
1	D	339	GLN
1	D	350	GLN
1	D	351	LEU
1	D	359	SER
1	D	360	THR
1	D	364	GLU
1	D	369	SER
1	D	372	LEU
1	D	373	GLU

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Mol	Chain	Res	Type
1	D	377	SER
1	D	384	GLN
1	D	392	ILE
1	D	393	GLN
1	D	404	THR
1	D	411	TYR
1	D	424	LEU
1	D	450	SER
1	D	455	VAL
1	D	473	VAL
1	D	477	VAL
1	D	478	GLU
1	D	485	ASP
1	D	490	ARG
1	D	506	LYS
1	D	510	GLN
1	E	3	HIS
1	E	25	ARG
1	E	35	MET
1	E	39	SER
1	E	41	GLU
1	E	42	THR
1	E	65	ILE
1	E	66	PHE
1	E	68	HIS
1	E	70	LYS
1	E	78	GLU
1	E	93	SER
1	E	116	GLU
1	E	122	ILE
1	E	125	MET
1	E	133	ARG
1	E	136	ASN
1	E	141	THR
1	E	149	MET
1	E	154	ILE
1	E	157	LEU
1	E	166	VAL
1	E	175	GLN
1	E	179	LEU
1	E	200	THR
1	E	204	TRP

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Mol	Chain	Res	Type
1	E	209	THR
1	E	225	VAL
1	E	234	THR
1	E	243	THR
1	E	248	ASN
1	E	251	THR
1	E	263	LYS
1	E	269	MET
1	E	271	VAL
1	E	278	MET
1	E	290	LEU
1	E	298	ILE
1	E	306	ARG
1	E	308	GLU
1	E	309	ARG
1	E	326	TYR
1	E	343	SER
1	E	363	LYS
1	E	364	GLU
1	E	372	LEU
1	E	374	VAL
1	E	378	SER
1	E	385	GLU
1	E	388	LEU
1	E	405	ASP
1	E	408	VAL
1	E	410	THR
1	E	413	ARG
1	E	433	ILE
1	E	438	GLN
1	E	451	TRP
1	E	464	LEU
1	E	473	VAL
1	E	478	GLU
1	E	479	LEU
1	E	493	THR
1	E	494	GLU
1	E	496	ARG
1	E	502	GLN
1	E	506	LYS
1	E	508	LYS
1	F	3	HIS

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Mol	Chain	Res	Type
1	F	13	ILE
1	F	25	ARG
1	F	35	MET
1	F	39	SER
1	F	41	GLU
1	F	42	THR
1	F	63	HIS
1	F	65	ILE
1	F	66	PHE
1	F	68	HIS
1	F	70	LYS
1	F	93	SER
1	F	109	ASN
1	F	116	GLU
1	F	121	CYS
1	F	122	ILE
1	F	125	MET
1	F	133	ARG
1	F	136	ASN
1	F	141	THR
1	F	149	MET
1	F	154	ILE
1	F	157	LEU
1	F	166	VAL
1	F	169	VAL
1	F	175	GLN
1	F	179	LEU
1	F	200	THR
1	F	204	TRP
1	F	209	THR
1	F	225	VAL
1	F	234	THR
1	F	248	ASN
1	F	251	THR
1	F	271	VAL
1	F	278	MET
1	F	281	GLN
1	F	286	LEU
1	F	290	LEU
1	F	295	THR
1	F	298	ILE
1	F	303	ARG

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Mol	Chain	Res	Type
1	F	306	ARG
1	F	308	GLU
1	F	309	ARG
1	F	343	SER
1	F	363	LYS
1	F	364	GLU
1	F	372	LEU
1	F	374	VAL
1	F	382	VAL
1	F	385	GLU
1	F	388	LEU
1	F	393	GLN
1	F	405	ASP
1	F	408	VAL
1	F	410	THR
1	F	438	GLN
1	F	443	TRP
1	F	451	TRP
1	F	473	VAL
1	F	478	GLU
1	F	479	LEU
1	F	493	THR
1	F	494	GLU
1	F	496	ARG
1	F	497	LEU
1	F	502	GLN
1	F	506	LYS
1	F	508	LYS
1	G	6	ILE
1	G	10	VAL
1	G	13	ILE
1	G	18	THR
1	G	24	LYS
1	G	36	ILE
1	G	41	GLU
1	G	42	THR
1	G	57	LEU
1	G	64	VAL
1	G	65	ILE
1	G	84	ASP
1	G	87	TYR
1	G	92	ILE

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Mol	Chain	Res	Type
1	G	107	GLN
1	G	108	ASN
1	G	111	SER
1	G	112	MET
1	G	116	GLU
1	G	119	VAL
1	G	142	PHE
1	G	143	ASP
1	G	147	VAL
1	G	150	MET
1	G	152	THR
1	G	158	PHE
1	G	159	MET
1	G	169	VAL
1	G	182	ARG
1	G	183	VAL
1	G	193	THR
1	G	194	ASN
1	G	200	THR
1	G	204	TRP
1	G	207	ASN
1	G	209	THR
1	G	210	PHE
1	G	222	TRP
1	G	223	ILE
1	G	248	ASN
1	G	249	ASN
1	G	252	VAL
1	G	254	LEU
1	G	256	ASP
1	G	258	THR
1	G	269	MET
1	G	271	VAL
1	G	272	ASP
1	G	279	ASN
1	G	281	GLN
1	G	286	LEU
1	G	294	SER
1	G	308	GLU
1	G	309	ARG
1	G	316	LEU
1	G	320	GLU

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Mol	Chain	Res	Type
1	G	326	TYR
1	G	331	PHE
1	G	332	SER
1	G	337	TYR
1	G	341	GLU
1	G	351	LEU
1	G	361	GLU
1	G	363	LYS
1	G	364	GLU
1	G	385	GLU
1	G	387	ILE
1	G	393	GLN
1	G	398	THR
1	G	402	LYS
1	G	408	VAL
1	G	411	TYR
1	G	424	LEU
1	G	445	ARG
1	G	453	TYR
1	G	455	VAL
1	G	477	VAL
1	G	478	GLU
1	G	485	ASP
1	G	490	ARG
1	G	491	GLN
1	G	492	ASN
1	G	510	GLN
1	H	6	ILE
1	H	10	VAL
1	H	13	ILE
1	H	24	LYS
1	H	36	ILE
1	H	41	GLU
1	H	57	LEU
1	H	64	VAL
1	H	65	ILE
1	H	70	LYS
1	H	77	ASP
1	H	84	ASP
1	H	87	TYR
1	H	92	ILE
1	H	94	TYR

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Mol	Chain	Res	Type
1	H	107	GLN
1	H	108	ASN
1	H	111	SER
1	H	112	MET
1	H	116	GLU
1	H	118	GLN
1	H	143	ASP
1	H	147	VAL
1	H	152	THR
1	H	158	PHE
1	H	169	VAL
1	H	183	VAL
1	H	193	THR
1	H	194	ASN
1	H	200	THR
1	H	203	ASN
1	H	204	TRP
1	H	209	THR
1	H	210	PHE
1	H	223	ILE
1	H	235	ARG
1	H	248	ASN
1	H	249	ASN
1	H	252	VAL
1	H	254	LEU
1	H	256	ASP
1	H	271	VAL
1	H	272	ASP
1	H	274	LEU
1	H	279	ASN
1	H	286	LEU
1	H	294	SER
1	H	308	GLU
1	H	309	ARG
1	H	316	LEU
1	H	326	TYR
1	H	331	PHE
1	H	337	TYR
1	H	341	GLU
1	H	351	LEU
1	H	358	GLN
1	H	361	GLU

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Mol	Chain	Res	Type
1	H	363	LYS
1	H	364	GLU
1	H	378	SER
1	H	385	GLU
1	H	387	ILE
1	H	393	GLN
1	H	398	THR
1	H	402	LYS
1	H	408	VAL
1	H	411	TYR
1	H	419	TYR
1	H	424	LEU
1	H	443	TRP
1	H	453	TYR
1	H	455	VAL
1	H	477	VAL
1	H	478	GLU
1	H	485	ASP
1	H	490	ARG
1	H	491	GLN
1	H	492	ASN
1	H	510	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	175	GLN
1	A	296	HIS
1	A	339	GLN
1	A	350	GLN
1	A	458	GLN
1	B	163	ASN
1	B	175	GLN
1	B	296	HIS
1	B	350	GLN
1	B	458	GLN
1	C	163	ASN
1	C	175	GLN
1	C	296	HIS
1	C	339	GLN
1	C	350	GLN

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Mol	Chain	Res	Type
1	C	458	GLN
1	D	63	HIS
1	D	175	GLN
1	D	296	HIS
1	D	339	GLN
1	D	458	GLN
1	E	68	HIS
1	E	175	GLN
1	E	207	ASN
1	E	339	GLN
1	E	412	HIS
1	F	63	HIS
1	F	109	ASN
1	F	175	GLN
1	F	194	ASN
1	F	207	ASN
1	F	279	ASN
1	F	339	GLN
1	F	412	HIS
1	G	28	GLN
1	G	339	GLN
1	G	383	ASN
1	G	412	HIS
1	G	492	ASN
1	H	28	GLN
1	H	90	GLN
1	H	194	ASN
1	H	203	ASN
1	H	339	GLN
1	H	383	ASN
1	H	393	GLN
1	H	412	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	601	-	48,58,58	1.88	10 (20%)	54,89,89	2.82	19 (35%)
3	GDU	A	602	-	29,38,38	1.76	5 (17%)	43,58,58	1.72	7 (16%)
2	FAD	B	601	-	48,58,58	1.90	12 (25%)	54,89,89	2.52	15 (27%)
3	GDU	B	602	-	29,38,38	1.75	6 (20%)	43,58,58	2.11	10 (23%)
2	FAD	C	601	-	48,58,58	2.03	13 (27%)	54,89,89	2.90	17 (31%)
3	GDU	C	602	-	29,38,38	1.81	5 (17%)	43,58,58	1.75	8 (18%)
2	FAD	D	601	-	48,58,58	2.11	13 (27%)	54,89,89	2.75	15 (27%)
3	GDU	D	602	-	29,38,38	1.83	5 (17%)	43,58,58	1.93	9 (20%)
2	FAD	E	601	-	48,58,58	2.03	13 (27%)	54,89,89	2.35	17 (31%)
3	GDU	E	602	-	29,38,38	1.73	5 (17%)	43,58,58	1.74	7 (16%)
2	FAD	F	601	-	48,58,58	1.95	11 (22%)	54,89,89	2.53	18 (33%)
3	GDU	F	602	-	29,38,38	1.74	5 (17%)	43,58,58	1.89	10 (23%)
2	FAD	G	601	-	48,58,58	2.76	17 (35%)	54,89,89	2.65	17 (31%)
2	FAD	H	601	-	48,58,58	2.13	13 (27%)	54,89,89	2.58	20 (37%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	A	601	-	1/1/9/9	2/30/50/50	0/6/6/6
3	GDU	A	602	-	-	0/19/59/59	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	601	-	-	2/30/50/50	0/6/6/6
3	GDU	B	602	-	-	0/19/59/59	0/3/3/3
2	FAD	C	601	-	-	0/30/50/50	0/6/6/6
3	GDU	C	602	-	-	0/19/59/59	0/3/3/3
2	FAD	D	601	-	-	0/30/50/50	0/6/6/6
3	GDU	D	602	-	-	0/19/59/59	0/3/3/3
2	FAD	E	601	-	-	0/30/50/50	0/6/6/6
3	GDU	E	602	-	-	0/19/59/59	0/3/3/3
2	FAD	F	601	-	1/1/9/9	0/30/50/50	0/6/6/6
3	GDU	F	602	-	-	0/19/59/59	0/3/3/3
2	FAD	G	601	-	-	0/30/50/50	0/6/6/6
2	FAD	H	601	-	-	0/30/50/50	0/6/6/6

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	FAD	C1'-N10	-9.53	1.38	1.48
2	G	601	FAD	C2B-C3B	-6.09	1.36	1.53
2	G	601	FAD	C10-N10	-5.53	1.32	1.39
2	G	601	FAD	C9A-C5X	-5.43	1.31	1.42
2	H	601	FAD	C2B-C3B	-5.04	1.39	1.53
2	C	601	FAD	C2B-C3B	-4.79	1.40	1.53
2	E	601	FAD	C2B-C3B	-4.72	1.40	1.53
2	F	601	FAD	C2B-C3B	-4.71	1.40	1.53
2	H	601	FAD	C1'-N10	-4.63	1.43	1.48
2	D	601	FAD	C10-N10	-4.63	1.33	1.39
2	D	601	FAD	C2B-C3B	-4.58	1.40	1.53
2	B	601	FAD	C2B-C3B	-4.56	1.41	1.53
2	A	601	FAD	C2B-C3B	-4.52	1.41	1.53
2	D	601	FAD	C1'-N10	-4.18	1.44	1.48
2	G	601	FAD	C9A-N10	-4.17	1.33	1.38
3	A	602	GDU	C4'-C3'	-4.10	1.41	1.52
2	C	601	FAD	C1'-N10	-4.05	1.44	1.48
2	G	601	FAD	O3'-C3'	-4.01	1.33	1.43
2	E	601	FAD	C10-N10	-3.97	1.34	1.39
2	G	601	FAD	O4B-C1B	-3.95	1.36	1.41
3	D	602	GDU	C4'-C3'	-3.93	1.42	1.52
3	C	602	GDU	C4'-C3'	-3.90	1.42	1.52
2	F	601	FAD	C10-N10	-3.87	1.34	1.39
2	C	601	FAD	C10-N10	-3.79	1.34	1.39
2	G	601	FAD	C4'-C3'	-3.73	1.45	1.53
3	E	602	GDU	C3D-C2D	-3.63	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	FAD	C1'-N10	-3.62	1.44	1.48
2	A	601	FAD	C10-N10	-3.61	1.35	1.39
2	H	601	FAD	C10-N10	-3.56	1.35	1.39
3	D	602	GDU	C3D-C2D	-3.53	1.43	1.53
3	B	602	GDU	C3D-C2D	-3.48	1.43	1.53
3	F	602	GDU	C4'-C3'	-3.47	1.43	1.52
2	D	601	FAD	C5'-C4'	-3.44	1.46	1.51
2	H	601	FAD	C5'-C4'	-3.44	1.46	1.51
2	H	601	FAD	O2'-C2'	-3.43	1.35	1.43
3	B	602	GDU	C4'-C3'	-3.39	1.43	1.52
3	C	602	GDU	C3D-C2D	-3.37	1.44	1.53
3	A	602	GDU	C3D-C2D	-3.34	1.44	1.53
3	E	602	GDU	C4'-C3'	-3.34	1.43	1.52
2	H	601	FAD	C9A-N10	-3.34	1.34	1.38
3	F	602	GDU	C3D-C2D	-3.26	1.44	1.53
2	G	601	FAD	C8-C7	-3.22	1.32	1.41
2	E	601	FAD	O2'-C2'	-3.19	1.36	1.43
2	G	601	FAD	C4X-C10	-3.19	1.35	1.41
2	C	601	FAD	O2'-C2'	-3.18	1.36	1.43
2	D	601	FAD	O2'-C2'	-3.14	1.36	1.43
2	A	601	FAD	O2'-C2'	-3.10	1.36	1.43
2	F	601	FAD	O2'-C2'	-3.08	1.36	1.43
2	B	601	FAD	C9A-N10	-3.06	1.34	1.38
3	D	602	GDU	C3D-C4D	-3.01	1.44	1.53
2	B	601	FAD	O2'-C2'	-2.92	1.36	1.43
2	E	601	FAD	C5'-C4'	-2.85	1.47	1.51
2	D	601	FAD	C9A-N10	-2.82	1.34	1.38
2	F	601	FAD	C5'-C4'	-2.79	1.47	1.51
3	C	602	GDU	C3D-C4D	-2.79	1.45	1.53
2	C	601	FAD	C5'-C4'	-2.77	1.47	1.51
2	D	601	FAD	PA-O1A	-2.77	1.41	1.51
3	F	602	GDU	C3D-C4D	-2.76	1.45	1.53
2	C	601	FAD	PA-O1A	-2.75	1.41	1.51
3	A	602	GDU	C3D-C4D	-2.72	1.45	1.53
2	E	601	FAD	C9A-N10	-2.67	1.35	1.38
2	A	601	FAD	PA-O1A	-2.67	1.41	1.51
2	G	601	FAD	O3B-C3B	-2.66	1.36	1.43
2	F	601	FAD	C1'-N10	-2.65	1.45	1.48
2	B	601	FAD	C1'-N10	-2.64	1.45	1.48
2	B	601	FAD	PA-O1A	-2.62	1.41	1.51
3	E	602	GDU	C3D-C4D	-2.61	1.46	1.53
3	B	602	GDU	C3D-C4D	-2.58	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	601	FAD	PA-O1A	-2.58	1.41	1.51
2	B	601	FAD	C10-N10	-2.53	1.36	1.39
2	C	601	FAD	C9A-N10	-2.50	1.35	1.38
2	E	601	FAD	PA-O1A	-2.49	1.42	1.51
2	H	601	FAD	PA-O1A	-2.44	1.42	1.51
2	H	601	FAD	C9A-C5X	-2.41	1.37	1.42
2	C	601	FAD	O4B-C1B	-2.38	1.38	1.41
2	A	601	FAD	O4B-C1B	-2.38	1.38	1.41
2	B	601	FAD	C5'-C4'	-2.37	1.48	1.51
2	G	601	FAD	C5X-N5	-2.33	1.31	1.35
2	B	601	FAD	C9A-C5X	-2.32	1.38	1.42
2	A	601	FAD	C5'-C4'	-2.30	1.48	1.51
2	D	601	FAD	O4B-C1B	-2.28	1.38	1.41
2	H	601	FAD	O4B-C1B	-2.27	1.38	1.41
2	F	601	FAD	O4B-C1B	-2.27	1.38	1.41
2	C	601	FAD	O4B-C4B	-2.26	1.39	1.45
2	E	601	FAD	O4B-C4B	-2.23	1.39	1.45
2	F	601	FAD	O4B-C4B	-2.21	1.39	1.45
2	A	601	FAD	O4B-C4B	-2.20	1.39	1.45
2	D	601	FAD	O4B-C4B	-2.19	1.40	1.45
2	E	601	FAD	O4B-C1B	-2.12	1.38	1.41
2	B	601	FAD	O4B-C4B	-2.10	1.40	1.45
3	B	602	GDU	PB-O3B	-2.10	1.54	1.60
2	G	601	FAD	C5A-N7A	-2.08	1.32	1.39
2	D	601	FAD	C9A-C5X	-2.08	1.38	1.42
2	G	601	FAD	C6-C5X	-2.08	1.38	1.41
2	E	601	FAD	C3B-C4B	-2.05	1.47	1.53
2	H	601	FAD	O4B-C4B	-2.03	1.40	1.45
2	C	601	FAD	C9A-C5X	-2.00	1.38	1.42
3	A	602	GDU	O5'-C5'	2.05	1.49	1.44
2	E	601	FAD	C6A-N6A	2.15	1.41	1.34
2	H	601	FAD	C6A-N6A	2.16	1.41	1.34
3	B	602	GDU	O5'-C5'	2.20	1.49	1.44
2	C	601	FAD	C6A-N6A	2.21	1.41	1.34
2	F	601	FAD	C6A-N6A	2.24	1.41	1.34
2	A	601	FAD	C6A-N6A	2.24	1.41	1.34
2	B	601	FAD	C6A-N6A	2.24	1.41	1.34
2	D	601	FAD	C6A-N6A	2.25	1.41	1.34
3	C	602	GDU	O5'-C5'	2.28	1.50	1.44
3	F	602	GDU	O5'-C5'	2.37	1.50	1.44
3	D	602	GDU	O5'-C5'	2.38	1.50	1.44
3	E	602	GDU	O5'-C5'	2.40	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	FAD	C7M-C7	2.41	1.55	1.51
2	D	601	FAD	C7M-C7	2.46	1.56	1.51
2	C	601	FAD	C7M-C7	2.50	1.56	1.51
2	E	601	FAD	C7M-C7	2.52	1.56	1.51
2	A	601	FAD	C7M-C7	2.52	1.56	1.51
2	H	601	FAD	C7M-C7	2.53	1.56	1.51
2	F	601	FAD	C7M-C7	2.55	1.56	1.51
2	G	601	FAD	C4-N3	2.79	1.38	1.33
2	G	601	FAD	C10-N1	2.83	1.40	1.35
2	G	601	FAD	C7M-C7	3.16	1.57	1.51
3	F	602	GDU	O4-C4	5.45	1.37	1.24
3	A	602	GDU	O4-C4	5.46	1.37	1.24
3	E	602	GDU	O4-C4	5.52	1.37	1.24
3	B	602	GDU	O4-C4	5.55	1.38	1.24
3	D	602	GDU	O4-C4	5.59	1.38	1.24
3	C	602	GDU	O4-C4	5.70	1.38	1.24
2	B	601	FAD	O4-C4	7.68	1.43	1.24
2	H	601	FAD	O4-C4	7.76	1.43	1.24
2	E	601	FAD	O4-C4	7.77	1.43	1.24
2	C	601	FAD	O4-C4	7.78	1.43	1.24
2	F	601	FAD	O4-C4	7.81	1.43	1.24
2	A	601	FAD	O4-C4	7.81	1.43	1.24
2	D	601	FAD	O4-C4	7.82	1.43	1.24

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	FAD	N3A-C2A-N1A	-11.03	120.45	128.89
2	C	601	FAD	N3A-C2A-N1A	-10.00	121.24	128.89
2	C	601	FAD	C4B-O4B-C1B	-9.93	98.80	109.72
2	F	601	FAD	N3A-C2A-N1A	-9.91	121.31	128.89
2	A	601	FAD	N3A-C2A-N1A	-9.85	121.36	128.89
2	E	601	FAD	N3A-C2A-N1A	-9.79	121.40	128.89
2	H	601	FAD	N3A-C2A-N1A	-9.55	121.58	128.89
2	D	601	FAD	N3A-C2A-N1A	-9.52	121.61	128.89
2	B	601	FAD	N3A-C2A-N1A	-9.50	121.62	128.89
2	B	601	FAD	C1'-N10-C9A	-7.79	110.11	118.86
2	C	601	FAD	C1B-N9A-C4A	-7.38	115.81	126.94
2	D	601	FAD	C1B-N9A-C4A	-6.68	116.87	126.94
2	D	601	FAD	C4B-O4B-C1B	-6.66	102.40	109.72
3	B	602	GDU	O5'-C1'-O3B	-6.01	103.44	111.36
2	D	601	FAD	C4-C4X-C10	-5.24	116.59	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C1B-N9A-C4A	-5.17	119.15	126.94
2	G	601	FAD	O3P-P-O5'	-4.95	89.80	102.94
2	G	601	FAD	C4X-C10-N10	-4.95	117.60	120.52
2	G	601	FAD	O5B-PA-O1A	-4.89	90.65	109.62
2	F	601	FAD	C1B-N9A-C4A	-4.84	119.64	126.94
2	A	601	FAD	C4B-O4B-C1B	-4.75	104.50	109.72
3	F	602	GDU	PB-O3A-PA	-4.68	119.60	132.73
2	H	601	FAD	C1'-N10-C9A	-4.60	113.70	118.86
3	D	602	GDU	PB-O3A-PA	-4.59	119.83	132.73
2	B	601	FAD	C1B-N9A-C4A	-4.47	120.20	126.94
2	H	601	FAD	C4B-O4B-C1B	-4.47	104.81	109.72
2	H	601	FAD	C1B-N9A-C4A	-4.32	120.42	126.94
2	H	601	FAD	P-O3P-PA	-4.31	120.63	132.73
2	C	601	FAD	C4-C4X-C10	-4.30	117.19	119.94
2	H	601	FAD	C4-C4X-C10	-4.30	117.19	119.94
3	A	602	GDU	PB-O3A-PA	-4.10	121.22	132.73
2	E	601	FAD	C2B-C1B-N9A	-4.06	108.09	114.29
2	E	601	FAD	C4-C4X-C10	-4.06	117.34	119.94
2	H	601	FAD	C2B-C1B-N9A	-3.95	108.26	114.29
3	C	602	GDU	PB-O3A-PA	-3.87	121.86	132.73
2	D	601	FAD	C4A-C5A-N7A	-3.86	105.93	109.48
3	E	602	GDU	PB-O3A-PA	-3.85	121.91	132.73
2	E	601	FAD	C1B-N9A-C4A	-3.85	121.13	126.94
2	G	601	FAD	O5'-P-O1P	-3.70	95.26	109.62
2	D	601	FAD	P-O3P-PA	-3.70	122.35	132.73
2	E	601	FAD	P-O3P-PA	-3.56	122.73	132.73
2	F	601	FAD	C4-C4X-C10	-3.54	117.68	119.94
2	F	601	FAD	P-O3P-PA	-3.47	123.00	132.73
2	A	601	FAD	C4A-C5A-N7A	-3.23	106.51	109.48
3	B	602	GDU	C1'-O5'-C5'	-3.17	107.60	113.75
2	C	601	FAD	C4A-C5A-N7A	-3.13	106.60	109.48
2	B	601	FAD	C4X-C10-N10	-3.05	118.72	120.52
2	B	601	FAD	C4-C4X-C10	-2.97	118.04	119.94
2	G	601	FAD	P-O3P-PA	-2.96	124.42	132.73
2	A	601	FAD	C4-C4X-C10	-2.95	118.05	119.94
3	B	602	GDU	PB-O3A-PA	-2.93	124.51	132.73
2	G	601	FAD	O3B-C3B-C2B	-2.91	102.36	111.83
3	B	602	GDU	O5'-C1'-C2'	-2.84	104.45	110.28
2	A	601	FAD	P-O3P-PA	-2.83	124.78	132.73
2	B	601	FAD	C2B-C1B-N9A	-2.80	110.01	114.29
2	F	601	FAD	C4A-C5A-N7A	-2.64	107.05	109.48
2	H	601	FAD	C4A-C5A-N7A	-2.61	107.07	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4X-C4-N3	-2.58	120.06	123.59
2	G	601	FAD	C8M-C8-C7	-2.58	115.07	120.73
2	G	601	FAD	C4B-O4B-C1B	-2.55	106.92	109.72
2	B	601	FAD	C4A-C5A-N7A	-2.55	107.14	109.48
2	D	601	FAD	C4X-C4-N3	-2.44	120.25	123.59
3	D	602	GDU	C4D-O4D-C1D	-2.41	107.07	109.72
2	G	601	FAD	C2B-C1B-N9A	-2.40	110.62	114.29
2	H	601	FAD	C4X-C10-N10	-2.36	119.13	120.52
2	E	601	FAD	C4X-C4-N3	-2.35	120.38	123.59
2	F	601	FAD	C4B-O4B-C1B	-2.33	107.16	109.72
2	E	601	FAD	C4A-C5A-N7A	-2.32	107.35	109.48
2	C	601	FAD	C4X-C4-N3	-2.31	120.43	123.59
2	F	601	FAD	C4X-C4-N3	-2.26	120.50	123.59
2	A	601	FAD	C6-C5X-N5	-2.25	116.07	118.96
2	F	601	FAD	C2B-C1B-N9A	-2.24	110.86	114.29
2	E	601	FAD	C4B-O4B-C1B	-2.24	107.26	109.72
2	B	601	FAD	P-O3P-PA	-2.22	126.48	132.73
2	H	601	FAD	C4X-C4-N3	-2.07	120.75	123.59
2	G	601	FAD	C4X-C4-N3	-2.04	120.79	123.59
2	C	601	FAD	P-O3P-PA	-2.01	127.07	132.73
2	E	601	FAD	C1'-N10-C9A	2.01	121.12	118.86
2	D	601	FAD	O2A-PA-O3P	2.01	114.23	105.09
3	F	602	GDU	C2D-C3D-C4D	2.02	106.76	102.61
2	F	601	FAD	O3P-PA-O5B	2.04	108.36	102.94
3	D	602	GDU	O3A-PB-O3B	2.07	109.58	103.63
3	F	602	GDU	C1'-O5'-C5'	2.08	117.79	113.75
2	E	601	FAD	O3P-PA-O5B	2.11	108.54	102.94
2	H	601	FAD	O3P-P-O5'	2.12	108.55	102.94
2	A	601	FAD	O2P-P-O3P	2.12	114.73	105.09
2	C	601	FAD	C5X-C9A-N10	2.17	119.27	117.62
2	B	601	FAD	O2'-C2'-C1'	2.17	115.28	109.94
3	F	602	GDU	O4D-C1D-N1	2.22	112.77	108.08
2	H	601	FAD	C4X-N5-C5X	2.23	119.33	116.76
2	F	601	FAD	C4-C4X-N5	2.23	121.43	118.72
3	C	602	GDU	O5D-C5D-C4D	2.23	117.36	109.12
3	F	602	GDU	O3A-PB-O3B	2.32	110.31	103.63
3	C	602	GDU	O3A-PB-O3B	2.35	110.39	103.63
3	C	602	GDU	O4D-C1D-N1	2.37	113.07	108.08
2	H	601	FAD	O3P-PA-O5B	2.37	109.22	102.94
3	B	602	GDU	O4D-C1D-N1	2.37	113.08	108.08
2	D	601	FAD	C5X-C9A-N10	2.39	119.44	117.62
2	D	601	FAD	C1'-C2'-C3'	2.42	116.75	109.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	GDU	O3A-PA-O5D	2.44	109.42	102.94
2	F	601	FAD	C1'-C2'-C3'	2.44	116.81	109.82
3	E	602	GDU	O5D-C5D-C4D	2.47	118.22	109.12
2	E	601	FAD	O5B-C5B-C4B	2.48	118.26	109.12
3	E	602	GDU	O3A-PB-O3B	2.48	110.77	103.63
2	H	601	FAD	O5B-C5B-C4B	2.48	118.28	109.12
2	F	601	FAD	O5B-C5B-C4B	2.49	118.30	109.12
2	C	601	FAD	O5B-C5B-C4B	2.56	118.54	109.12
3	A	602	GDU	O5'-C1'-C2'	2.57	115.54	110.28
2	F	601	FAD	C5X-C9A-N10	2.57	119.58	117.62
2	G	601	FAD	C4-N3-C2	2.59	117.48	115.25
2	A	601	FAD	C4-C4X-N5	2.60	121.88	118.72
2	C	601	FAD	O3P-P-O5'	2.61	109.85	102.94
3	A	602	GDU	O5D-C5D-C4D	2.65	118.89	109.12
2	A	601	FAD	C1'-C2'-C3'	2.66	117.43	109.82
2	B	601	FAD	O2'-C2'-C3'	2.66	115.71	109.02
3	F	602	GDU	O5D-C5D-C4D	2.70	119.07	109.12
3	B	602	GDU	O5D-C5D-C4D	2.72	119.15	109.12
2	E	601	FAD	C5X-C9A-N10	2.75	119.71	117.62
3	E	602	GDU	O3A-PA-O5D	2.78	110.31	102.94
2	A	601	FAD	C4X-C10-N10	2.78	122.16	120.52
3	D	602	GDU	O5'-C1'-C2'	2.83	116.09	110.28
3	A	602	GDU	O3A-PB-O3B	2.88	111.91	103.63
3	D	602	GDU	O4D-C1D-N1	2.91	114.21	108.08
3	C	602	GDU	O3A-PA-O5D	2.92	110.69	102.94
2	E	601	FAD	C4-C4X-N5	2.98	122.33	118.72
2	C	601	FAD	C1'-C2'-C3'	2.99	118.38	109.82
2	H	601	FAD	O2'-C2'-C3'	3.06	116.71	109.02
3	C	602	GDU	C3'-C4'-C5'	3.07	115.56	110.20
2	C	601	FAD	O3P-PA-O5B	3.08	111.11	102.94
2	C	601	FAD	O2'-C2'-C1'	3.09	117.53	109.94
2	A	601	FAD	O3P-PA-O5B	3.09	111.14	102.94
3	B	602	GDU	O5'-C5'-C4'	3.10	115.50	109.68
3	B	602	GDU	O3A-PA-O5D	3.14	111.26	102.94
2	H	601	FAD	C5X-C9A-N10	3.14	120.01	117.62
2	H	601	FAD	O2'-C2'-C1'	3.19	117.78	109.94
3	C	602	GDU	O5'-C5'-C4'	3.22	115.72	109.68
2	C	601	FAD	C4-C4X-N5	3.22	122.63	118.72
3	D	602	GDU	C1'-O5'-C5'	3.28	120.10	113.75
3	A	602	GDU	C1'-C2'-C3'	3.28	116.43	109.97
2	H	601	FAD	C4-C4X-N5	3.31	122.74	118.72
2	G	601	FAD	O4B-C1B-N9A	3.35	115.11	108.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	GDU	C3'-C4'-C5'	3.36	116.06	110.20
2	A	601	FAD	O5B-C5B-C4B	3.39	121.63	109.12
3	F	602	GDU	O3A-PA-O5D	3.45	112.09	102.94
2	G	601	FAD	O2P-P-O5'	3.49	126.05	108.46
2	F	601	FAD	O4B-C1B-N9A	3.51	115.44	108.10
2	D	601	FAD	C4-C4X-N5	3.52	123.00	118.72
3	E	602	GDU	O5'-C5'-C4'	3.55	116.34	109.68
2	B	601	FAD	O5B-C5B-C4B	3.61	122.44	109.12
2	E	601	FAD	O4B-C1B-N9A	3.66	115.75	108.10
2	B	601	FAD	O3P-PA-O5B	3.68	112.70	102.94
2	C	601	FAD	O2'-C2'-C3'	3.75	118.44	109.02
2	E	601	FAD	O2'-C2'-C3'	3.83	118.65	109.02
2	B	601	FAD	O4B-C1B-N9A	4.05	116.58	108.10
2	G	601	FAD	O2A-PA-O3P	4.08	123.60	105.09
3	B	602	GDU	C3'-C4'-C5'	4.12	117.38	110.20
2	G	601	FAD	O5B-C5B-C4B	4.18	124.53	109.12
2	D	601	FAD	O2'-C2'-C3'	4.20	119.58	109.02
3	D	602	GDU	O5'-C5'-C4'	4.21	117.58	109.68
3	F	602	GDU	O5'-C5'-C4'	4.23	117.63	109.68
2	D	601	FAD	O2'-C2'-C1'	4.31	120.53	109.94
2	F	601	FAD	O2'-C2'-C3'	4.31	119.85	109.02
3	F	602	GDU	C3'-C4'-C5'	4.31	117.71	110.20
2	G	601	FAD	O2P-P-O3P	4.33	124.75	105.09
2	E	601	FAD	O2'-C2'-C1'	4.42	120.80	109.94
2	A	601	FAD	O2'-C2'-C3'	4.61	120.61	109.02
2	A	601	FAD	O2'-C2'-C1'	4.66	121.40	109.94
2	B	601	FAD	C4-N3-C2	4.86	119.45	115.25
3	E	602	GDU	C3'-C4'-C5'	4.89	118.73	110.20
2	F	601	FAD	O2'-C2'-C1'	5.15	122.61	109.94
2	F	601	FAD	C4-N3-C2	5.17	119.71	115.25
2	H	601	FAD	C4-N3-C2	5.18	119.72	115.25
2	A	601	FAD	O4B-C1B-N9A	5.33	119.25	108.10
2	A	601	FAD	C4-N3-C2	5.33	119.85	115.25
2	B	601	FAD	C5X-C9A-N10	5.35	121.69	117.62
2	H	601	FAD	O4B-C1B-N9A	5.45	119.50	108.10
2	E	601	FAD	C4-N3-C2	5.53	120.02	115.25
3	A	602	GDU	C4-N3-C2	5.64	119.72	114.14
2	C	601	FAD	C4-N3-C2	5.65	120.13	115.25
3	E	602	GDU	C4-N3-C2	5.66	119.74	114.14
3	F	602	GDU	C4-N3-C2	5.92	120.01	114.14
2	D	601	FAD	O4B-C1B-N9A	5.98	120.61	108.10
3	D	602	GDU	C4-N3-C2	6.22	120.30	114.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	FAD	C4-N3-C2	6.26	120.66	115.25
2	F	601	FAD	C1'-N10-C9A	6.30	125.94	118.86
3	C	602	GDU	C4-N3-C2	6.33	120.42	114.14
2	C	601	FAD	O4B-C1B-N9A	6.50	121.70	108.10
3	B	602	GDU	C4-N3-C2	7.08	121.15	114.14
2	A	601	FAD	C1'-N10-C9A	8.55	128.46	118.86

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	601	FAD	C2'
2	A	601	FAD	C2'

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	C2'-C1'-N10-C10
2	B	601	FAD	C2'-C1'-N10-C9A

There are no ring outliers.

14 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	FAD	10	0
3	A	602	GDU	9	0
2	B	601	FAD	14	0
3	B	602	GDU	15	0
2	C	601	FAD	12	0
3	C	602	GDU	9	0
2	D	601	FAD	22	0
3	D	602	GDU	4	0
2	E	601	FAD	20	0
3	E	602	GDU	14	0
2	F	601	FAD	14	0
3	F	602	GDU	8	0
2	G	601	FAD	13	0
2	H	601	FAD	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	509/509 (100%)	-0.28	4 (0%) 87 75	22, 64, 110, 167	0
1	B	509/509 (100%)	-0.30	7 (1%) 78 60	24, 64, 106, 166	0
1	C	509/509 (100%)	-0.28	7 (1%) 78 60	29, 65, 108, 170	0
1	D	509/509 (100%)	-0.27	6 (1%) 81 64	27, 65, 109, 172	0
1	E	509/509 (100%)	-0.39	1 (0%) 95 91	22, 62, 99, 156	0
1	F	509/509 (100%)	-0.34	3 (0%) 90 80	23, 59, 99, 151	0
1	G	509/509 (100%)	-0.44	0 100 100	14, 61, 93, 126	0
1	H	509/509 (100%)	-0.42	1 (0%) 95 91	22, 63, 94, 132	1 (0%)
All	All	4072/4072 (100%)	-0.34	29 (0%) 89 78	14, 63, 104, 172	1 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	TRP	5.4
1	C	183	VAL	4.9
1	B	183	VAL	4.5
1	F	207	ASN	4.4
1	B	204	TRP	4.4
1	A	204	TRP	4.3
1	C	184	ALA	4.0
1	D	205	GLY	3.7
1	D	186	PRO	3.7
1	D	204	TRP	3.4
1	A	205	GLY	3.4
1	C	201	ALA	3.2
1	C	202	GLY	2.9
1	D	206	PRO	2.8
1	A	184	ALA	2.8
1	F	206	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	182	ARG	2.5
1	B	186	PRO	2.3
1	H	206	PRO	2.3
1	B	205	GLY	2.2
1	B	184	ALA	2.2
1	E	200	THR	2.1
1	F	185	ALA	2.1
1	C	185	ALA	2.1
1	B	180	GLY	2.1
1	D	184	ALA	2.1
1	D	207	ASN	2.1
1	C	205	GLY	2.0
1	A	104	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	FAD	B	601	53/53	0.97	0.20	-0.08	18,64,87,92	0
3	GDU	A	602	36/36	0.95	0.23	-0.37	30,108,162,203	0
2	FAD	F	601	53/53	0.98	0.18	-0.40	12,67,90,107	0
2	FAD	C	601	53/53	0.98	0.18	-0.42	0,49,83,94	0
3	GDU	B	602	36/36	0.96	0.21	-0.49	42,114,153,160	0
2	FAD	D	601	53/53	0.99	0.18	-0.52	0,57,88,102	0
2	FAD	E	601	53/53	0.98	0.17	-0.54	14,57,97,102	0
2	FAD	H	601	53/53	0.97	0.16	-0.60	20,79,102,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	FAD	A	601	53/53	0.98	0.17	-0.60	6,57,87,95	0
3	GDU	C	602	36/36	0.96	0.18	-0.68	25,103,142,180	0
3	GDU	E	602	36/36	0.94	0.18	-0.76	22,92,139,142	0
3	GDU	F	602	36/36	0.95	0.17	-0.77	28,101,153,194	0
2	FAD	G	601	53/53	0.98	0.15	-0.86	0,57,86,102	0
3	GDU	D	602	36/36	0.95	0.15	-1.18	35,99,135,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.