Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 01:56 pm GMT

PDB ID	:	1H6V
Title	:	Mammalian thioredoxin reductase
Authors	:	Sandalova, T.; Zhong, L.; Lindqvist, Y.; Holmgren, A.; Schneider, G.
Deposited on	:	2001-06-27
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

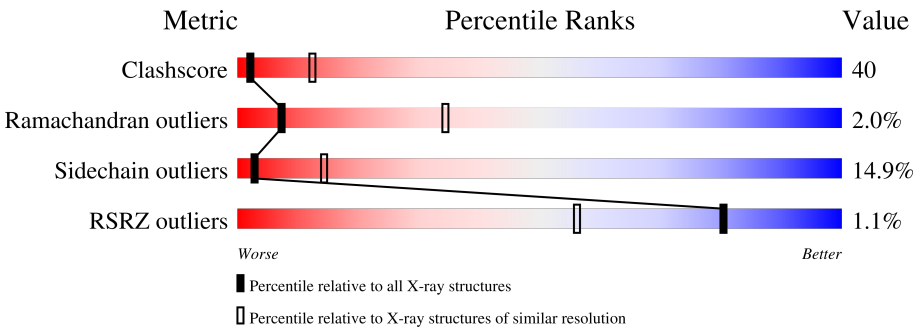
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	499	40% 49% 8% •
1	B	499	44% 43% 10% • •
1	C	499	3% 28% 54% 14% • •
1	D	499	% 44% 40% 11% • •
1	E	499	% 47% 41% 9% • •
1	F	499	% 44% 43% 10% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 23075 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 THIOREDOXIN REDUCTASE.

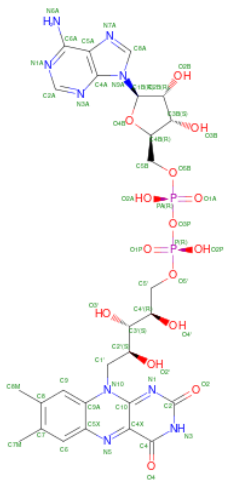
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	490	3764	2391	635	716	22	0	0	0
1	B	487	3753	2387	633	713	20	0	0	0
1	C	482	3707	2356	627	704	20	0	0	0
1	D	487	3753	2387	633	713	20	0	0	0
1	E	491	3773	2397	637	717	22	0	0	0
1	F	490	3764	2391	635	716	22	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	52	ASN	ARG	conflict	UNP O89049
B	52	ASN	ARG	conflict	UNP O89049
C	52	ASN	ARG	conflict	UNP O89049
D	52	ASN	ARG	conflict	UNP O89049
E	52	ASN	ARG	conflict	UNP O89049
F	52	ASN	ARG	conflict	UNP O89049
A	497	CYS	SEL	engineered mutation	UNP O89049
B	497	CYS	SEL	engineered mutation	UNP O89049
C	497	CYS	SEL	engineered mutation	UNP O89049
D	497	CYS	SEL	engineered mutation	UNP O89049
E	497	CYS	SEL	engineered mutation	UNP O89049

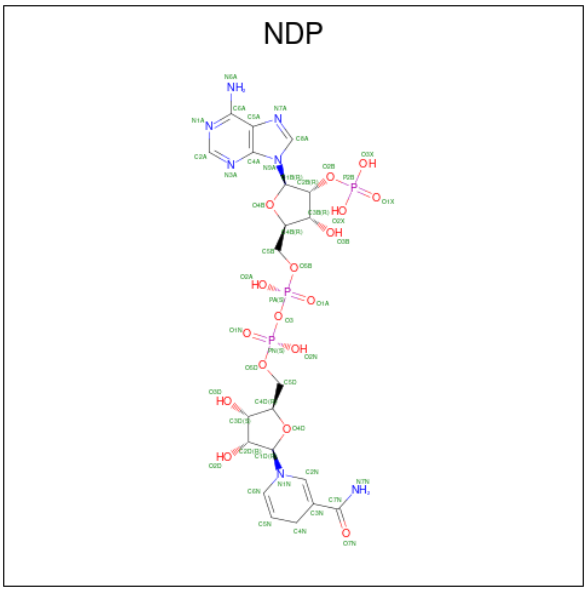
- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD



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

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	39	15	5	16	3	0	0
3	B	1	39	15	5	16	3	0	0
3	C	1	39	15	5	16	3	0	0
3	D	1	39	15	5	16	3	0	0
3	E	1	39	15	5	16	3	0	0
3	F	1	39	15	5	16	3	0	0

- Molecule 4 is water.

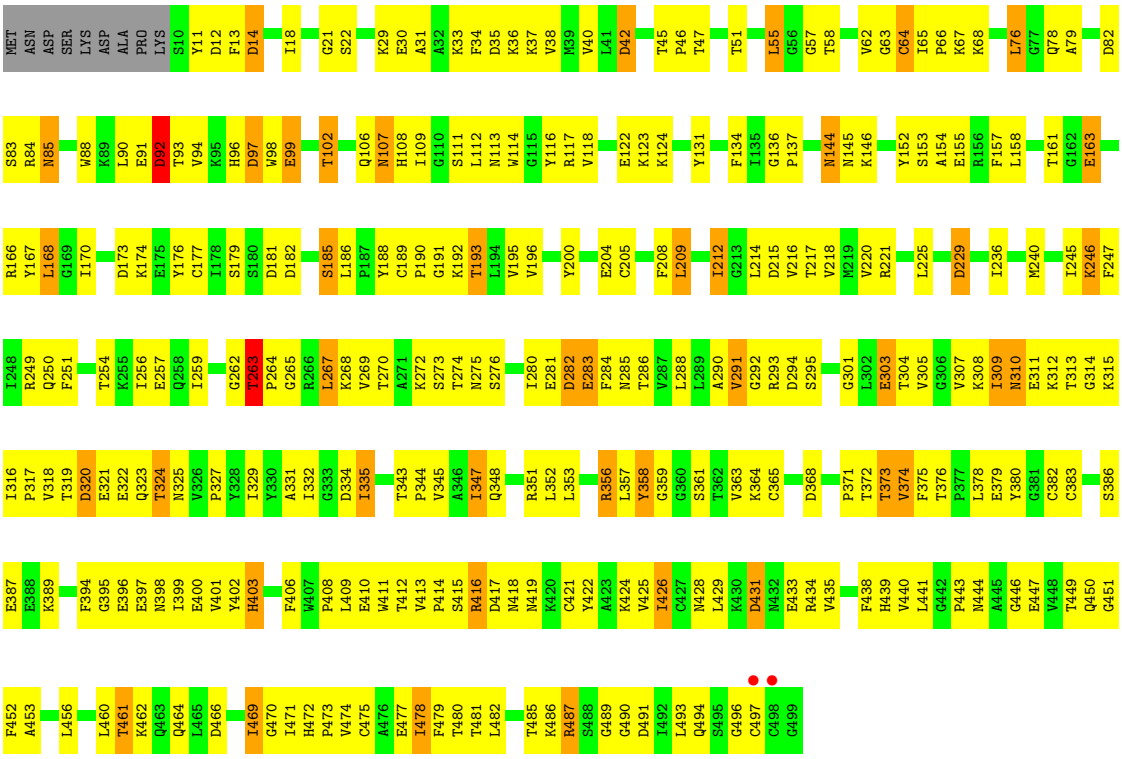
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	3	3	3	0	0
4	D	1	1	1	0	0
4	E	2	2	2	0	0
4	F	1	1	1	0	0

3 Residue-property plots (i)

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

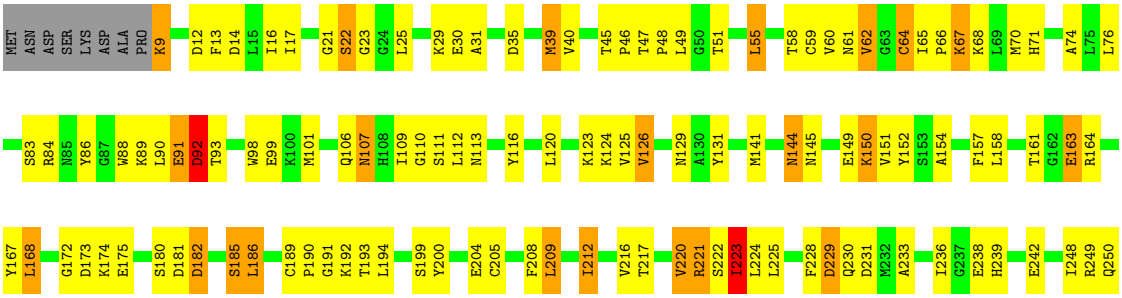
• Molecule 1: THIOREDOXIN REDUCTASE

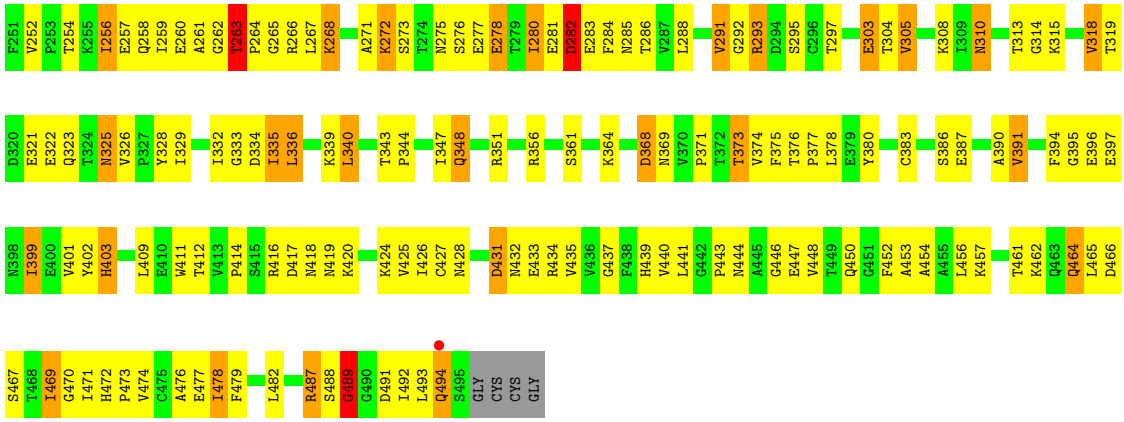
Chain A: 40% 49% 8% •



• Molecule 1: THIOREDOXIN REDUCTASE

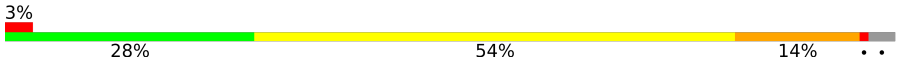
Chain B: 44% 43% 10% ••

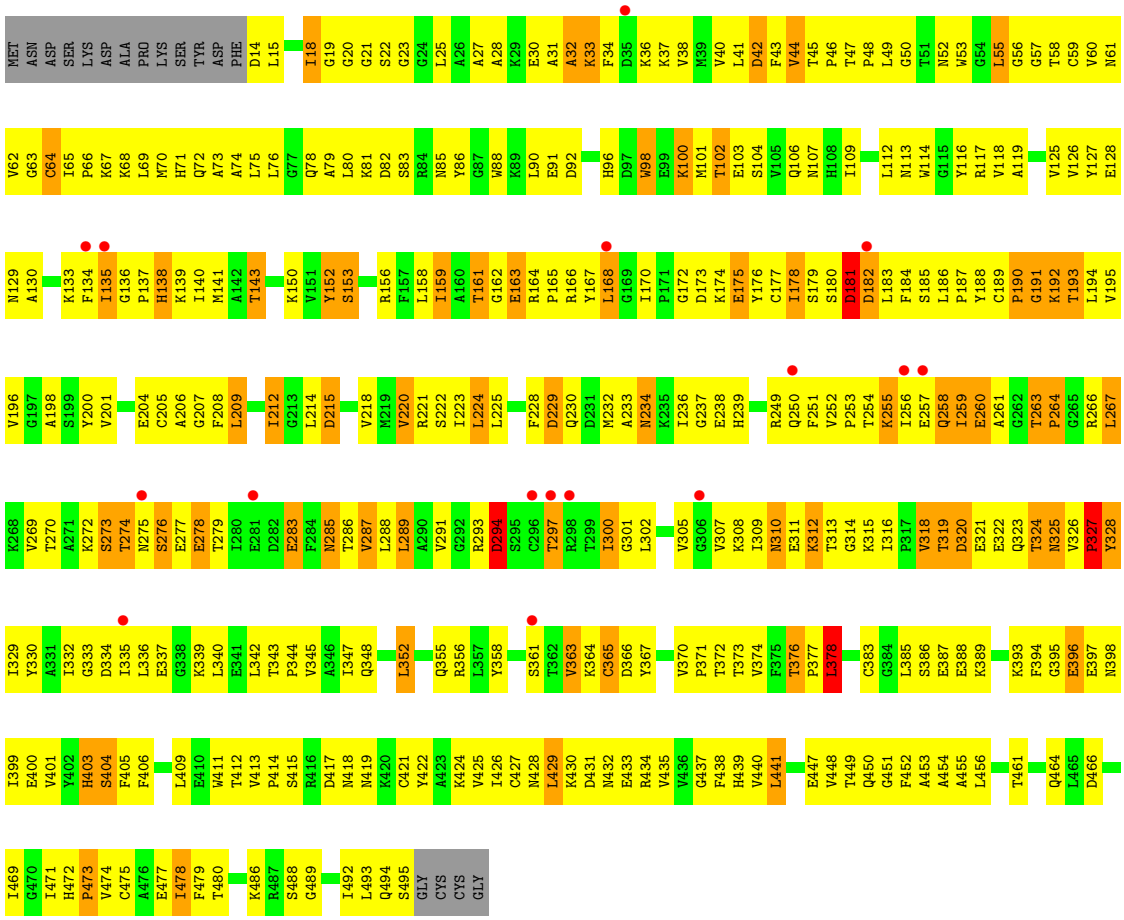




• Molecule 1: THIOREDOXIN REDUCTASE

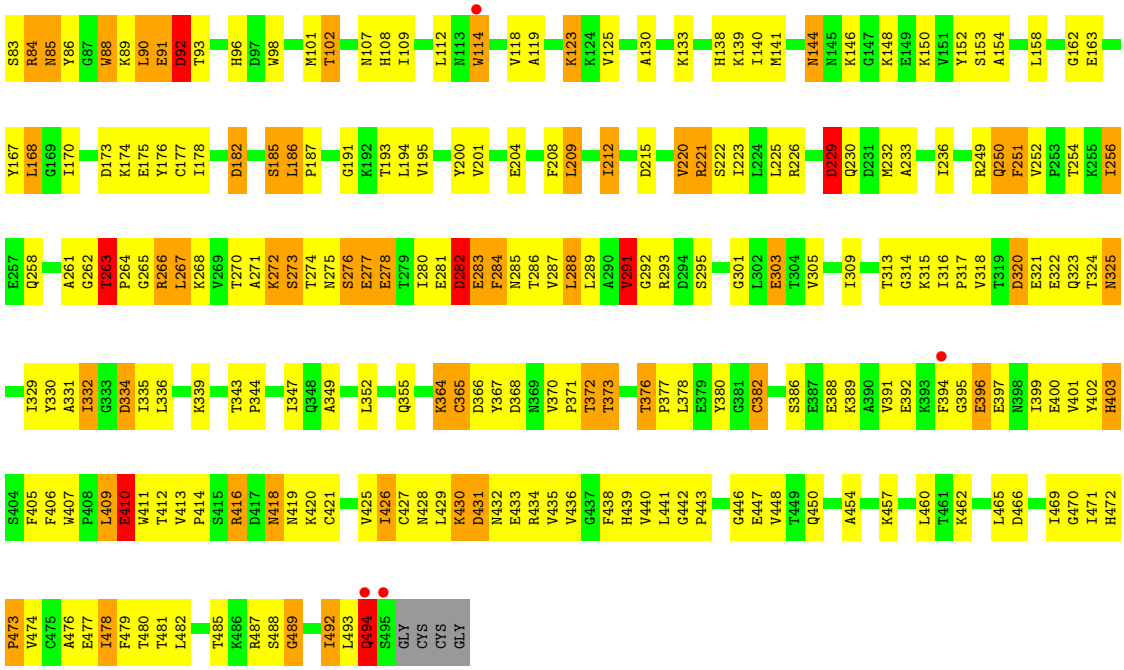
Chain C:





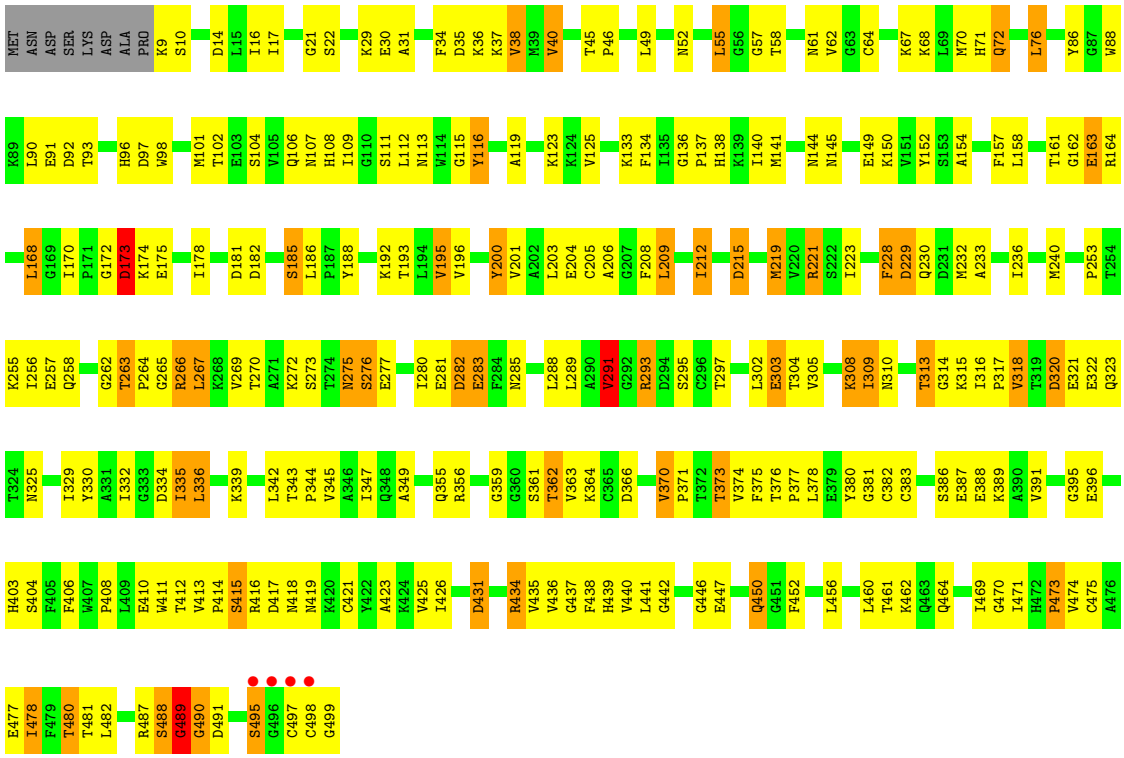
• Molecule 1: THIOREDOXIN REDUCTASE

Chain D:



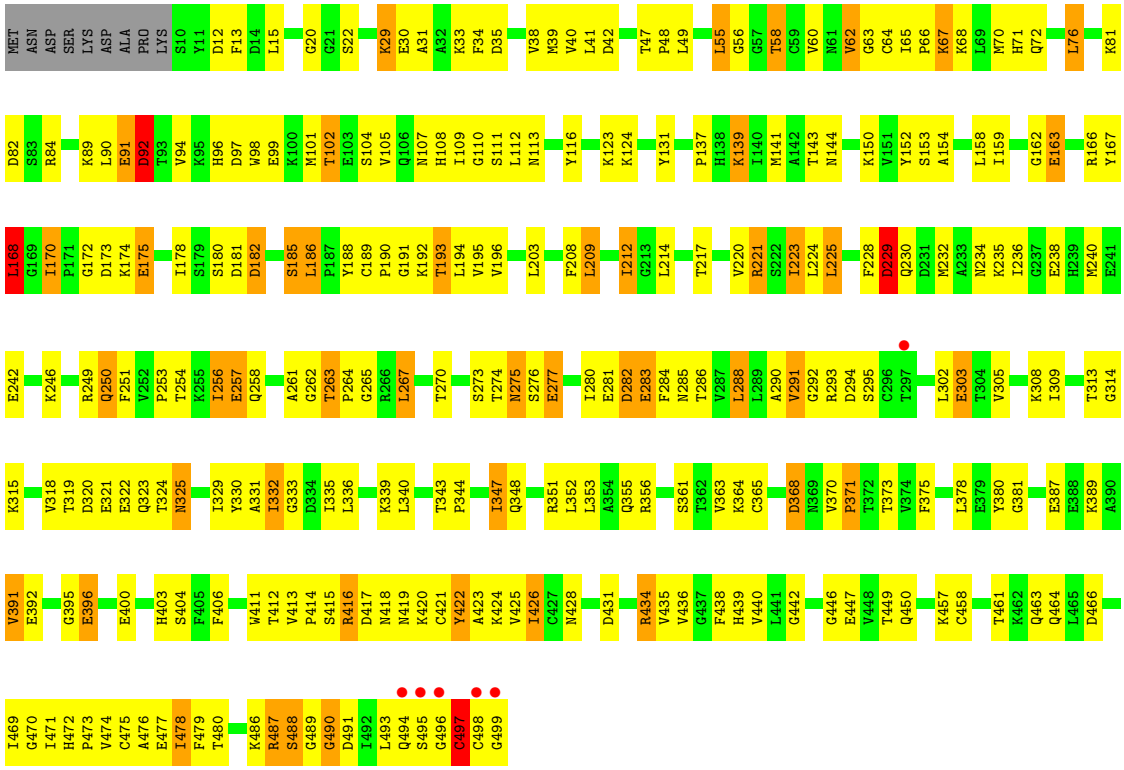
- Molecule 1: THIOREDOXIN REDUCTASE

Chain E:



- Molecule 1: THIOREDOXIN REDUCTASE

Chain F:


MET ASN ASP SER LYS ASP ALA PRO LYS S10 Y11 D12 F13 D14 L15 G20 G21 S22 K29 E30 A31 A32 K33 F34 D35 V38 M39 V40 L41 D42 T47 P48 L49 L55 G56 G57 T58 C59 V60 N61 V62 G63 C64 I65 P66 K67 K68 L69 M70 H71 Q72 L76 K81
D82 S83 R84 K89 L90 E91 D92 T93 V94 K95 H96 D97 W98 E99 K100 M101 T102 E103 S104 V105 Q106 N107 H108 I109 G110 S111 L112 N113 Y116 K123 K124 Y131 P137 H138 K139 I140 M141 A142 T143 N144 K150 V151 Y152 S153 A154 L158 I159 G162 E163 R166 Y167
L168 G169 I170 P171 G172 D173 K174 E175 I178 S179 S180 D181 D182 S185 L186 P187 Y188 C189 P190 G191 K192 T193 L194 V195 V196 L203 F208 L209 I212 G213 L214 T217 V220 R221 S222 I223 L224 L225 F228 D229 Q230 D231 M232 A233 N234 K235 I236 G237 E238 H239 M240 E241
E242 K246 R249 Q250 F251 V252 P253 T254 K255 I256 E257 Q258 A261 G262 T263 P264 G265 R266 L267 T270 S273 T274 N275 S276 E277 I280 E281 D282 E283 F284 N285 T286 V287 L288 L289 A290 V291 G292 R293 D294 S295 C296 T297 L302 E303 T304 V305 K308 I309 T313 G314
K315 V318 T319 D320 E321 E322 Q323 T324 N325 I329 Y330 A331 I332 G333 D334 I335 L336 K339 L340 T343 P344 I347 Q348 R351 L352 L353 A354 Q355 R356 S361 T362 V363 K364 C365 D368 N369 V370 P371 T372 T373 V374 F375 L378 E379 Y380 G381 E387 E388 K389 A390
V391 E392 G395 E396 E400 H403 S404 F405 F406 W411 T412 V413 P414 S415 R416 D417 N418 N419 K420 C421 Y422 A423 K424 V425 I426 C427 N428 D431 R434 V435 V436 G437 F438 H439 V440 L441 G442 G446 E447 V448 T449 Q450 K457 C458 T461 K462 Q463 Q464 L465 D466
I469 G470 I471 H472 P473 V474 C475 A476 E477 I478 F479 T480 K486 R487 S488 G489 G490 D491 I492 L493 Q494 S495 G496 G497 C498 G499

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	78.92Å 140.46Å 170.83Å 90.00° 94.64° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.86 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-3.00) 92.5 (29.86-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.224 , 0.263 0.257 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	61.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 4.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	23075	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.92	0/3838	1.07	15/5193 (0.3%)
1	B	0.90	0/3827	1.04	14/5178 (0.3%)
1	C	0.82	1/3779 (0.0%)	1.03	15/5114 (0.3%)
1	D	0.97	3/3827 (0.1%)	1.08	16/5178 (0.3%)
1	E	0.99	2/3847 (0.1%)	1.11	16/5204 (0.3%)
1	F	0.80	0/3838	1.03	14/5193 (0.3%)
All	All	0.90	6/22956 (0.0%)	1.06	90/31060 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	489	GLY	C-O	-6.05	1.14	1.23
1	D	410	GLU	CD-OE1	5.80	1.32	1.25
1	D	114	TRP	CB-CG	-5.08	1.41	1.50
1	C	300	ILE	C-O	-5.07	1.13	1.23
1	D	88	TRP	CB-CG	-5.03	1.41	1.50
1	E	116	TYR	CG-CD2	-5.01	1.32	1.39

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	82	ASP	CB-CG-OD2	9.47	126.82	118.30
1	F	229	ASP	CB-CG-OD2	9.21	126.59	118.30
1	F	417	ASP	CB-CG-OD2	8.16	125.65	118.30
1	E	282	ASP	CB-CG-OD2	7.91	125.42	118.30
1	F	466	ASP	CB-CG-OD2	7.83	125.35	118.30
1	A	368	ASP	CB-CG-OD2	7.77	125.30	118.30
1	E	320	ASP	CB-CG-OD2	7.54	125.08	118.30
1	D	35	ASP	CB-CG-OD2	7.46	125.02	118.30
1	E	417	ASP	CB-CG-OD2	7.45	125.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	334	ASP	CB-CG-OD2	7.34	124.91	118.30
1	A	417	ASP	CB-CG-OD2	7.34	124.91	118.30
1	F	368	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	182	ASP	CB-CG-OD2	7.03	124.63	118.30
1	D	14	ASP	CB-CG-OD2	7.02	124.62	118.30
1	E	173	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	35	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	417	ASP	CB-CG-OD2	6.71	124.34	118.30
1	A	320	ASP	CB-CG-OD2	6.65	124.28	118.30
1	F	495	SER	C-N-CA	-6.64	108.35	122.30
1	C	42	ASP	CB-CG-OD2	6.64	124.28	118.30
1	C	92	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	282	ASP	CB-CG-OD2	6.50	124.15	118.30
1	B	466	ASP	CB-CG-OD2	6.45	124.11	118.30
1	F	35	ASP	CB-CG-OD2	6.33	123.99	118.30
1	E	229	ASP	CB-CG-OD2	6.31	123.97	118.30
1	D	215	ASP	CB-CG-OD2	6.24	123.92	118.30
1	C	14	ASP	CB-CG-OD2	6.20	123.88	118.30
1	B	223	ILE	CG1-CB-CG2	-6.19	97.78	111.40
1	E	181	ASP	CB-CG-OD2	6.17	123.86	118.30
1	F	182	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	92	ASP	CB-CG-OD2	6.11	123.80	118.30
1	D	274	THR	CB-CA-C	-6.10	95.12	111.60
1	F	371	PRO	N-CD-CG	-6.09	94.06	103.20
1	E	293	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	F	496	GLY	N-CA-C	6.04	128.20	113.10
1	F	168	LEU	CA-CB-CG	6.04	129.19	115.30
1	A	97	ASP	CB-CG-OD2	5.96	123.66	118.30
1	A	182	ASP	CB-CG-OD2	5.93	123.63	118.30
1	E	431	ASP	CB-CG-OD2	5.91	123.62	118.30
1	E	490	GLY	N-CA-C	-5.88	98.39	113.10
1	C	294	ASP	CB-CG-OD2	5.85	123.56	118.30
1	D	282	ASP	CB-CG-OD2	5.85	123.56	118.30
1	E	97	ASP	CB-CG-OD2	5.84	123.55	118.30
1	B	340	LEU	CA-CB-CG	5.83	128.71	115.30
1	B	489	GLY	N-CA-C	5.79	127.58	113.10
1	D	80	LEU	CB-CG-CD1	-5.75	101.23	111.00
1	B	182	ASP	CB-CG-OD2	5.72	123.45	118.30
1	D	368	ASP	CB-CG-OD2	5.67	123.40	118.30
1	C	229	ASP	CB-CG-OD2	5.58	123.32	118.30
1	E	313	THR	OG1-CB-CG2	-5.58	97.16	110.00
1	D	273	SER	N-CA-CB	5.54	118.81	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	263	THR	N-CA-C	-5.50	96.16	111.00
1	C	215	ASP	CB-CG-OD2	5.47	123.22	118.30
1	A	42	ASP	CB-CG-OD2	5.46	123.22	118.30
1	A	431	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	181	ASP	CB-CG-OD2	5.44	123.19	118.30
1	F	497	CYS	N-CA-C	-5.43	96.35	111.00
1	C	181	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	65	ILE	CG1-CB-CG2	-5.36	99.62	111.40
1	C	378	LEU	CA-CB-CG	5.35	127.60	115.30
1	E	488	SER	CB-CA-C	-5.35	99.94	110.10
1	A	290	ALA	CB-CA-C	5.35	118.12	110.10
1	D	229	ASP	CB-CG-OD2	5.33	123.09	118.30
1	B	126	VAL	CB-CA-C	-5.32	101.29	111.40
1	F	92	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	368	ASP	CB-CG-OD2	5.29	123.06	118.30
1	D	320	ASP	CB-CG-OD2	5.29	123.06	118.30
1	E	366	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	18	ILE	CG1-CB-CG2	-5.25	99.85	111.40
1	C	466	ASP	CB-CG-OD2	5.24	123.02	118.30
1	B	14	ASP	CB-CG-OD2	5.23	123.01	118.30
1	C	320	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	489	GLY	N-CA-C	5.21	126.13	113.10
1	A	215	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	431	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	12	ASP	CB-CG-OD2	5.17	122.96	118.30
1	F	62	VAL	CB-CA-C	-5.17	101.57	111.40
1	A	490	GLY	N-CA-C	-5.14	100.24	113.10
1	D	293	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	B	224	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	E	195	VAL	CB-CA-C	-5.13	101.66	111.40
1	C	327	PRO	N-CA-C	5.12	125.42	112.10
1	B	431	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	466	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	320	ASP	CB-CG-OD2	5.08	122.87	118.30
1	E	495	SER	C-N-CA	-5.08	111.64	122.30
1	A	374	VAL	CB-CA-C	-5.05	101.80	111.40
1	D	466	ASP	CB-CG-OD2	5.04	122.84	118.30
1	C	417	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	182	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3764	0	3764	309	0
1	B	3753	0	3763	287	0
1	C	3707	0	3721	463	0
1	D	3753	0	3761	294	0
1	E	3773	0	3777	257	0
1	F	3764	0	3764	300	0
2	A	53	0	31	5	0
2	B	53	0	31	10	0
2	C	53	0	31	17	0
2	D	53	0	31	4	0
2	E	53	0	31	3	0
2	F	53	0	31	5	0
3	A	39	0	18	2	0
3	B	39	0	18	8	0
3	C	39	0	18	6	0
3	D	39	0	18	6	0
3	E	39	0	18	1	0
3	F	39	0	18	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	3	0	0	2	0
4	D	1	0	0	0	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	23075	0	22844	1832	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 (1832) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:TRP:NE1	1:C:190:PRO:HD2	1.54	1.21
1:C:98:TRP:CD1	1:C:189:CYS:HA	1.76	1.20
1:D:477:GLU:O	1:D:480:THR:HG22	1.49	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD13	1:C:441:LEU:HD11	1.13	1.12
1:C:98:TRP:CZ3	1:C:102:THR:HG23	1.85	1.12
1:F:478:ILE:N	1:F:478:ILE:HD12	1.62	1.11
1:C:98:TRP:HZ3	1:C:102:THR:HG23	1.00	1.11
1:C:18:ILE:HG13	1:C:18:ILE:O	1.47	1.10
1:D:303:GLU:OE1	1:D:303:GLU:N	1.84	1.10
1:B:371:PRO:HG3	1:B:453:ALA:HB2	1.34	1.10
1:F:168:LEU:HB3	1:F:170:ILE:HG23	1.35	1.04
1:A:263:THR:OG1	1:A:264:PRO:CD	2.07	1.03
1:C:72:GLN:HE21	1:D:410:GLU:HB3	1.18	1.01
1:C:378:LEU:HD13	1:C:441:LEU:CD1	1.90	1.01
1:C:172:GLY:HA2	1:C:175:GLU:HG3	1.36	1.01
1:C:255:LYS:HD2	1:C:270:THR:OG1	1.62	1.00
1:D:251:PHE:HD1	1:D:273:SER:HB2	1.22	1.00
1:C:320:ASP:O	1:C:364:LYS:HG3	1.62	1.00
1:A:98:TRP:NE1	1:A:102:THR:HG21	1.76	0.99
1:C:98:TRP:HE3	1:C:102:THR:HG1	1.02	0.99
1:A:378:LEU:HG	1:A:441:LEU:HD11	1.44	0.98
1:D:320:ASP:OD2	1:D:364:LYS:NZ	1.97	0.98
1:E:289:LEU:O	1:E:291:VAL:HG22	1.64	0.97
1:B:67:LYS:HE2	1:B:204:GLU:OE1	1.63	0.97
1:F:238:GLU:O	1:F:242:GLU:HG3	1.64	0.97
1:E:263:THR:HB	1:E:264:PRO:HD3	1.46	0.97
1:F:426:ILE:HD11	1:F:436:VAL:HG23	1.43	0.97
1:F:361:SER:OG	1:F:363:VAL:HG23	1.63	0.96
1:D:325:ASN:HD22	1:D:325:ASN:N	1.62	0.96
1:C:272:LYS:HE3	1:C:276:SER:HA	1.49	0.95
1:C:461:THR:OG1	1:C:464:GLN:HG3	1.66	0.94
1:C:426:ILE:HG22	1:C:437:GLY:HA3	1.49	0.94
1:A:478:ILE:HD12	1:A:478:ILE:N	1.83	0.94
1:E:256:ILE:HD13	1:E:269:VAL:HG22	1.47	0.94
1:A:114:TRP:HB3	1:D:114:TRP:NE1	1.82	0.93
1:C:224:LEU:H	1:C:224:LEU:HD12	1.32	0.93
1:A:263:THR:OG1	1:A:264:PRO:HD3	1.66	0.93
1:A:353:LEU:HD12	1:A:356:ARG:HH21	1.34	0.92
1:B:65:ILE:HG22	1:B:66:PRO:HD3	1.51	0.92
1:C:403:HIS:CE1	1:C:492:ILE:HD11	2.05	0.92
1:A:348:GLN:HE22	1:A:351:ARG:NH1	1.66	0.92
1:C:258:GLN:HE22	1:C:261:ALA:HB2	1.33	0.92
1:E:303:GLU:OE2	1:E:304:THR:HG23	1.69	0.92
1:F:192:LYS:N	1:F:285:ASN:HD22	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:331:ALA:O	1:F:332:ILE:HD12	1.70	0.91
1:F:478:ILE:HD12	1:F:478:ILE:H	1.24	0.91
1:B:426:ILE:HG12	1:B:437:GLY:HA3	1.52	0.91
1:D:325:ASN:H	1:D:325:ASN:ND2	1.64	0.91
1:C:418:ASN:ND2	1:C:419:ASN:H	1.68	0.90
1:D:389:LYS:NZ	1:D:392:GLU:OE1	2.05	0.90
1:A:78:GLN:HE21	1:A:416:ARG:NH1	1.69	0.90
1:B:67:LYS:HE2	1:B:204:GLU:CD	1.90	0.90
1:B:193:THR:HG22	1:B:286:THR:HB	1.51	0.89
1:C:220:VAL:HG21	1:C:249:ARG:NE	1.87	0.89
1:F:223:ILE:HD11	1:F:230:GLN:CD	1.93	0.89
1:E:497:CYS:SG	1:F:116:TYR:CE2	2.66	0.89
1:B:313:THR:O	1:B:315:LYS:N	2.04	0.89
1:F:313:THR:O	1:F:315:LYS:N	2.05	0.88
1:D:270:THR:HG22	1:D:280:ILE:HA	1.55	0.88
1:E:263:THR:CB	1:E:264:PRO:CD	2.51	0.88
1:F:191:GLY:O	1:F:193:THR:HG22	1.74	0.88
1:A:394:PHE:O	1:A:398:ASN:ND2	2.06	0.88
1:B:371:PRO:CG	1:B:453:ALA:CB	2.52	0.88
1:D:325:ASN:HD22	1:D:325:ASN:H	0.88	0.87
1:C:192:LYS:HE2	1:C:215:ASP:OD2	1.73	0.87
1:D:313:THR:O	1:D:315:LYS:N	2.06	0.87
1:A:318:VAL:CG1	1:A:322:GLU:HA	2.04	0.87
1:D:250:GLN:O	1:D:273:SER:CB	2.23	0.87
1:C:256:ILE:HD11	1:C:267:LEU:CD1	2.05	0.87
1:C:291:VAL:HG12	1:C:291:VAL:O	1.74	0.87
1:E:406:PHE:CZ	1:E:421:CYS:HB3	2.09	0.86
1:E:308:LYS:H	1:E:325:ASN:HD21	1.18	0.86
1:C:285:ASN:HD22	1:C:285:ASN:H	1.21	0.86
1:E:343:THR:HB	1:E:344:PRO:HD3	1.55	0.86
1:D:144:ASN:HD22	1:D:146:LYS:H	1.24	0.86
1:F:434:ARG:HH11	1:F:434:ARG:HG2	1.40	0.86
1:C:164:ARG:HB3	1:C:165:PRO:HD2	1.56	0.85
1:A:373:THR:HG23	1:B:471:ILE:HG21	1.58	0.85
1:B:262:GLY:O	1:B:263:THR:O	1.93	0.85
1:C:46:PRO:HB3	1:C:50:GLY:HA2	1.59	0.85
1:E:144:ASN:OD1	1:E:145:ASN:N	2.09	0.85
1:E:263:THR:OG1	1:E:264:PRO:HD2	1.75	0.85
1:B:192:LYS:H	1:B:285:ASN:HD22	1.25	0.85
1:C:96:HIS:HE1	1:D:86:TYR:O	1.58	0.85
1:E:434:ARG:HG2	1:E:434:ARG:HH11	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:VAL:HG11	1:A:322:GLU:HA	1.57	0.85
1:B:371:PRO:HG3	1:B:453:ALA:CB	2.06	0.85
1:B:371:PRO:CG	1:B:453:ALA:HB2	2.07	0.85
1:C:196:VAL:O	1:C:291:VAL:CG2	2.25	0.84
1:C:313:THR:OG1	1:C:315:LYS:HG3	1.77	0.84
1:A:66:PRO:HG3	1:A:109:ILE:HD11	1.59	0.84
1:B:66:PRO:HG3	1:B:109:ILE:HD11	1.59	0.84
1:C:96:HIS:CD2	1:C:212:ILE:HG13	2.11	0.84
1:F:325:ASN:ND2	1:F:325:ASN:H	1.73	0.84
1:A:220:VAL:HG21	1:A:249:ARG:HE	1.40	0.84
1:B:295:SER:HB3	1:B:335:ILE:HD12	1.57	0.84
1:A:308:LYS:H	1:A:325:ASN:ND2	1.75	0.83
1:D:407:TRP:CG	1:D:418:ASN:ND2	2.45	0.83
1:A:98:TRP:O	1:A:102:THR:HG23	1.79	0.83
1:F:478:ILE:N	1:F:478:ILE:CD1	2.39	0.83
1:C:196:VAL:HG12	1:C:291:VAL:HG21	1.59	0.83
1:C:447:GLU:OE2	1:D:474:VAL:HG13	1.78	0.83
1:A:493:LEU:O	1:A:494:GLN:HG2	1.79	0.83
1:B:131:TYR:CZ	2:B:600:FAD:N6A	2.46	0.83
1:F:223:ILE:HD11	1:F:230:GLN:NE2	1.94	0.83
1:F:275:ASN:ND2	1:F:275:ASN:O	2.12	0.83
1:E:232:MET:HE1	1:E:441:LEU:HB2	1.60	0.82
1:C:98:TRP:CZ3	1:C:102:THR:CG2	2.61	0.82
1:E:374:VAL:HG12	1:E:376:THR:HG23	1.58	0.82
1:C:185:SER:O	1:C:187:PRO:HD3	1.79	0.82
1:C:208:PHE:CE1	1:C:209:LEU:HD22	2.13	0.82
1:C:383:CYS:SG	1:C:456:LEU:HD12	2.18	0.82
1:E:313:THR:O	1:E:315:LYS:N	2.12	0.82
1:C:403:HIS:NE2	1:C:492:ILE:HD11	1.94	0.82
1:D:98:TRP:NE1	1:D:102:THR:HG21	1.94	0.82
1:E:263:THR:HB	1:E:264:PRO:CD	2.10	0.82
1:E:490:GLY:N	4:E:2002:HOH:O	2.11	0.82
1:D:144:ASN:ND2	1:D:146:LYS:H	1.78	0.82
1:A:99:GLU:HG2	1:D:146:LYS:HD3	1.59	0.81
1:D:52:ASN:HD22	1:D:52:ASN:N	1.78	0.81
1:A:65:ILE:HB	1:A:66:PRO:CD	2.09	0.81
1:A:353:LEU:HA	1:A:356:ARG:NH2	1.95	0.81
1:C:18:ILE:O	1:C:18:ILE:CG1	2.27	0.81
1:C:196:VAL:O	1:C:291:VAL:HG23	1.81	0.81
1:F:256:ILE:HD11	1:F:267:LEU:HB3	1.61	0.81
1:F:422:TYR:HD1	1:F:423:ALA:N	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:493:LEU:C	1:B:494:GLN:HG3	2.00	0.81
1:C:230:GLN:O	1:C:234:ASN:ND2	2.13	0.81
1:B:223:ILE:HG13	1:B:230:GLN:OE1	1.81	0.81
1:C:418:ASN:HD22	1:C:419:ASN:H	1.28	0.81
1:E:426:ILE:HG12	1:E:437:GLY:HA3	1.62	0.81
1:A:397:GLU:H	1:A:397:GLU:CD	1.81	0.81
1:D:251:PHE:HA	1:D:273:SER:HB2	1.61	0.81
1:F:469:ILE:N	1:F:469:ILE:HD12	1.95	0.80
1:A:295:SER:HB3	1:A:335:ILE:HD12	1.62	0.80
1:B:426:ILE:CG1	1:B:437:GLY:HA3	2.12	0.80
1:A:353:LEU:HD12	1:A:356:ARG:NH2	1.96	0.80
1:A:478:ILE:HD12	1:A:478:ILE:H	1.43	0.80
1:C:168:LEU:HD22	1:C:289:LEU:HD21	1.61	0.80
1:C:98:TRP:HZ3	1:C:102:THR:CG2	1.90	0.80
1:B:150:LYS:HG2	1:B:152:TYR:CE1	2.17	0.80
1:C:477:GLU:HA	1:D:450:GLN:NE2	1.96	0.80
1:D:114:TRP:HZ3	1:D:118:VAL:HG21	1.47	0.80
1:A:358:TYR:N	1:A:358:TYR:CD1	2.49	0.79
1:D:114:TRP:CZ3	1:D:118:VAL:HG21	2.17	0.79
1:D:251:PHE:HD1	1:D:273:SER:CB	1.94	0.79
1:E:173:ASP:OD1	1:E:174:LYS:N	2.16	0.79
1:A:308:LYS:H	1:A:325:ASN:HD21	1.28	0.79
1:A:272:LYS:HE3	1:A:276:SER:HA	1.64	0.79
1:C:318:VAL:HG13	1:C:319:THR:O	1.81	0.79
1:C:239:HIS:ND1	1:C:378:LEU:HB2	1.97	0.79
1:C:378:LEU:CD1	1:C:441:LEU:HD11	2.05	0.79
1:E:431:ASP:OD2	1:E:434:ARG:NH1	2.14	0.79
1:B:493:LEU:HD23	1:B:493:LEU:N	1.97	0.78
1:C:163:GLU:HB3	1:C:294:ASP:C	2.03	0.78
1:C:58:THR:O	1:C:63:GLY:N	2.16	0.78
1:E:150:LYS:HD3	1:E:152:TYR:OH	1.83	0.78
1:E:471:ILE:HG21	1:F:373:THR:HG23	1.66	0.78
1:A:67:LYS:NZ	1:A:204:GLU:OE1	2.16	0.78
1:C:310:ASN:ND2	1:C:312:LYS:H	1.82	0.78
1:E:320:ASP:OD2	1:E:364:LYS:NZ	2.15	0.78
1:F:422:TYR:CD1	1:F:423:ALA:N	2.52	0.78
1:F:313:THR:O	1:F:313:THR:OG1	1.94	0.78
1:C:106:GLN:O	1:C:109:ILE:HB	1.83	0.78
1:C:426:ILE:CG2	1:C:437:GLY:HA3	2.13	0.78
1:C:98:TRP:HD1	1:C:189:CYS:HA	1.45	0.78
1:C:472:HIS:HD2	1:C:477:GLU:OE2	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:CE	1:B:204:GLU:OE1	2.31	0.77
1:F:428:ASN:HD22	1:F:431:ASP:CB	1.96	0.77
1:A:418:ASN:HD22	1:A:419:ASN:H	1.33	0.77
1:F:305:VAL:HG11	1:F:329:ILE:HD11	1.66	0.77
1:B:291:VAL:HG22	3:B:601:NDP:C4A	2.15	0.77
1:C:67:LYS:HD3	1:C:204:GLU:HG2	1.66	0.77
1:A:262:GLY:O	1:A:263:THR:O	2.03	0.76
1:C:20:GLY:HA3	1:C:42:ASP:CG	2.06	0.76
1:C:98:TRP:HE1	1:C:190:PRO:HD2	1.45	0.76
1:E:371:PRO:HB2	1:F:471:ILE:HD11	1.67	0.76
1:F:192:LYS:H	1:F:285:ASN:HD22	1.31	0.76
1:D:51:THR:C	1:D:52:ASN:HD22	1.89	0.76
1:C:179:SER:H	1:C:182:ASP:HB2	1.49	0.76
1:D:168:LEU:HB3	1:D:170:ILE:HG23	1.66	0.76
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.51	0.76
1:D:473:PRO:HG2	1:D:473:PRO:O	1.84	0.76
1:F:493:LEU:O	1:F:494:GLN:HG2	1.85	0.76
1:D:407:TRP:HB2	1:D:418:ASN:HD21	1.51	0.76
1:C:161:THR:HG23	1:C:335:ILE:CD1	2.16	0.76
1:D:418:ASN:ND2	1:D:419:ASN:H	1.84	0.76
1:D:250:GLN:O	1:D:273:SER:HB2	1.85	0.75
1:F:20:GLY:N	1:F:42:ASP:OD1	2.15	0.75
1:F:380:TYR:OH	1:F:439:HIS:HD2	1.69	0.75
1:F:323:GLN:HA	1:F:330:TYR:CD1	2.20	0.75
1:B:373:THR:HG21	1:B:446:GLY:HA2	1.69	0.75
1:A:374:VAL:HG12	1:A:376:THR:HG23	1.68	0.75
1:A:378:LEU:HG	1:A:441:LEU:CD1	2.15	0.75
1:C:325:ASN:O	1:C:327:PRO:HD3	1.87	0.75
1:E:426:ILE:CG1	1:E:437:GLY:HA3	2.16	0.75
1:A:291:VAL:O	1:A:291:VAL:HG12	1.87	0.75
1:A:373:THR:HG21	1:A:446:GLY:HA2	1.66	0.74
1:A:418:ASN:ND2	1:A:419:ASN:H	1.84	0.74
1:D:291:VAL:HG13	1:D:291:VAL:O	1.87	0.74
1:C:263:THR:OG1	1:C:264:PRO:HD3	1.87	0.74
1:C:471:ILE:HG21	1:D:373:THR:HG23	1.69	0.74
1:E:192:LYS:H	1:E:285:ASN:HD22	1.35	0.74
1:F:373:THR:HG21	1:F:446:GLY:HA2	1.69	0.74
1:A:36:LYS:HG3	1:A:358:TYR:CD2	2.22	0.74
1:C:59:CYS:HA	1:C:63:GLY:HA3	1.69	0.74
1:E:374:VAL:CG1	1:E:376:THR:HG23	2.16	0.74
1:E:86:TYR:O	1:F:96:HIS:HE1	1.71	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:GLY:HA3	1:F:497:CYS:SG	2.27	0.74
1:D:418:ASN:HD22	1:D:419:ASN:H	1.33	0.74
1:B:192:LYS:N	1:B:285:ASN:HD22	1.86	0.74
1:E:272:LYS:HE2	1:E:276:SER:HA	1.70	0.74
1:F:110:GLY:HA2	1:F:113:ASN:HD22	1.52	0.74
1:B:65:ILE:CG2	1:B:66:PRO:HD3	2.18	0.74
1:C:98:TRP:CE2	1:C:190:PRO:HD2	2.23	0.73
1:C:163:GLU:OE2	1:C:334:ASP:HB3	1.88	0.73
1:C:256:ILE:HD11	1:C:267:LEU:HD13	1.68	0.73
1:A:471:ILE:HG21	1:B:373:THR:HG23	1.70	0.73
1:C:178:ILE:HD13	1:C:178:ILE:N	2.04	0.73
1:C:258:GLN:NE2	1:C:261:ALA:HB2	2.02	0.73
1:E:282:ASP:N	1:E:282:ASP:OD1	2.20	0.73
1:A:65:ILE:HB	1:A:66:PRO:HD2	1.71	0.73
1:C:220:VAL:HG23	1:C:249:ARG:HA	1.68	0.73
1:F:71:HIS:CD2	1:F:375:PHE:HB3	2.23	0.73
1:F:325:ASN:H	1:F:325:ASN:HD22	1.35	0.73
1:A:114:TRP:O	1:A:118:VAL:HG23	1.89	0.73
1:B:256:ILE:HD11	1:B:267:LEU:HD13	1.71	0.73
1:C:55:LEU:CD1	1:C:116:TYR:HB3	2.18	0.73
1:D:30:GLU:OE2	1:D:33:LYS:HE3	1.89	0.73
1:D:352:LEU:HD12	1:D:365:CYS:HB2	1.71	0.73
1:D:163:GLU:HB3	1:D:295:SER:HA	1.71	0.72
1:A:310:ASN:C	1:A:310:ASN:HD22	1.92	0.72
1:B:310:ASN:ND2	1:B:313:THR:H	1.87	0.72
1:F:39:MET:CE	1:F:41:LEU:HD21	2.20	0.72
1:B:39:MET:HB2	1:B:126:VAL:HB	1.72	0.72
1:C:343:THR:N	2:C:600:FAD:O3'	2.23	0.72
1:C:285:ASN:HD22	1:C:285:ASN:N	1.87	0.72
1:D:373:THR:HG21	1:D:446:GLY:HA2	1.69	0.72
1:D:394:PHE:HB2	1:D:399:ILE:HD11	1.70	0.72
1:D:119:ALA:O	1:D:123:LYS:HG3	1.88	0.72
1:B:191:GLY:O	1:B:193:THR:HG23	1.90	0.72
1:B:356:ARG:NH1	1:B:364:LYS:HA	2.05	0.72
1:C:188:TYR:CD2	1:C:263:THR:HG22	2.25	0.72
1:F:389:LYS:HD2	1:F:392:GLU:OE1	1.90	0.72
1:F:425:VAL:HG13	1:F:435:VAL:HG13	1.70	0.72
1:B:295:SER:HB3	1:B:335:ILE:CD1	2.19	0.72
1:C:178:ILE:HD13	1:C:178:ILE:H	1.54	0.72
1:E:404:SER:HB3	1:E:478:ILE:HD11	1.72	0.72
1:A:263:THR:OG1	1:A:264:PRO:HD2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:PHE:CD1	1:D:273:SER:HB2	2.15	0.71
1:E:410:GLU:OE2	1:F:68:LYS:NZ	2.22	0.71
1:A:189:CYS:SG	1:A:214:LEU:HD21	2.30	0.71
1:F:263:THR:HB	1:F:264:PRO:HD3	1.72	0.71
1:A:310:ASN:ND2	1:A:312:LYS:H	1.88	0.71
1:B:64:CYS:SG	2:B:600:FAD:C4X	2.78	0.71
1:D:82:ASP:OD2	1:D:416:ARG:NH1	2.23	0.71
1:B:403:HIS:CD2	1:B:492:ILE:HD13	2.25	0.71
1:C:309:ILE:HG22	1:C:316:ILE:HG12	1.71	0.71
1:A:167:TYR:CE2	1:A:174:LYS:HA	2.26	0.71
1:F:192:LYS:H	1:F:285:ASN:ND2	1.87	0.71
1:A:22:SER:OG	1:A:343:THR:HG23	1.90	0.71
1:A:379:GLU:O	1:A:441:LEU:HD12	1.91	0.71
1:D:67:LYS:NZ	1:D:204:GLU:OE1	2.21	0.71
1:C:19:GLY:HA2	2:C:600:FAD:N3A	2.05	0.71
1:B:281:GLU:O	1:B:282:ASP:C	2.29	0.71
1:C:425:VAL:HG13	1:C:435:VAL:HG13	1.71	0.71
1:E:373:THR:CG2	1:F:471:ILE:HG21	2.21	0.71
1:C:23:GLY:N	2:C:600:FAD:O1P	2.22	0.71
1:D:254:THR:HG23	1:D:271:ALA:HA	1.72	0.71
1:E:263:THR:OG1	1:E:264:PRO:CD	2.39	0.71
1:B:425:VAL:HG13	1:B:435:VAL:HG13	1.72	0.70
1:F:406:PHE:CE1	1:F:421:CYS:HB3	2.26	0.70
1:C:404:SER:HA	1:C:492:ILE:CG2	2.21	0.70
1:E:262:GLY:O	1:E:263:THR:O	2.09	0.70
1:B:282:ASP:N	1:B:282:ASP:OD1	2.23	0.70
1:E:461:THR:OG1	1:E:464:GLN:HG3	1.91	0.70
1:F:15:LEU:HB3	1:F:38:VAL:HG12	1.73	0.70
1:F:426:ILE:CD1	1:F:436:VAL:HG23	2.19	0.70
1:A:310:ASN:HD22	1:A:311:GLU:N	1.90	0.70
1:C:258:GLN:HE22	1:C:261:ALA:CB	2.03	0.70
1:F:256:ILE:HD12	1:F:257:GLU:N	2.07	0.70
1:F:426:ILE:HD11	1:F:436:VAL:CG2	2.21	0.70
1:D:431:ASP:O	1:D:432:ASN:HB2	1.92	0.70
1:A:267:LEU:HD22	1:A:267:LEU:N	2.07	0.70
1:B:163:GLU:HB3	1:B:295:SER:HA	1.73	0.70
1:C:477:GLU:HA	1:D:450:GLN:HE21	1.54	0.70
1:A:90:LEU:HD21	1:B:90:LEU:HD21	1.73	0.69
1:A:471:ILE:HD11	1:B:371:PRO:HB3	1.74	0.69
1:B:474:VAL:O	1:B:477:GLU:HG2	1.91	0.69
1:E:14:ASP:OD2	1:E:37:LYS:N	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LEU:HD11	1:A:332:ILE:CG1	2.21	0.69
1:D:400:GLU:OE2	1:D:487:ARG:HD2	1.92	0.69
1:B:291:VAL:HG22	3:B:601:NDP:N9A	2.07	0.69
1:B:401:VAL:HG22	1:B:426:ILE:HG22	1.72	0.69
1:C:67:LYS:HD3	1:C:204:GLU:CD	2.12	0.69
1:C:186:LEU:HD12	1:C:190:PRO:HG3	1.72	0.69
1:E:450:GLN:HE22	1:F:470:GLY:HA2	1.57	0.69
1:A:263:THR:O	1:A:265:GLY:N	2.25	0.69
1:E:289:LEU:O	1:E:291:VAL:CG2	2.40	0.69
1:C:21:GLY:O	1:C:25:LEU:HG	1.92	0.69
1:C:67:LYS:HD3	1:C:204:GLU:CG	2.22	0.69
1:C:438:PHE:CE2	1:C:452:PHE:CG	2.80	0.69
1:E:473:PRO:O	1:F:68:LYS:HE3	1.93	0.69
1:A:373:THR:CG2	1:B:471:ILE:HG21	2.23	0.69
1:A:470:GLY:HA2	1:B:450:GLN:HE22	1.57	0.69
1:C:256:ILE:HD11	1:C:267:LEU:HD12	1.72	0.69
1:F:223:ILE:CG1	1:F:230:GLN:NE2	2.56	0.69
1:C:220:VAL:CG2	1:C:249:ARG:HA	2.22	0.69
1:A:65:ILE:CB	1:A:66:PRO:CD	2.71	0.69
1:A:78:GLN:NE2	1:A:416:ARG:NH1	2.40	0.69
1:C:42:ASP:OD1	1:C:43:PHE:N	2.25	0.69
1:D:266:ARG:HD2	1:D:283:GLU:OE1	1.93	0.68
1:C:418:ASN:ND2	1:C:419:ASN:N	2.38	0.68
1:C:315:LYS:HD3	1:C:337:GLU:HA	1.75	0.68
1:D:96:HIS:CD2	1:D:212:ILE:HG13	2.29	0.68
1:D:400:GLU:HG2	1:D:429:LEU:HD11	1.74	0.68
1:C:20:GLY:HA3	1:C:42:ASP:OD2	1.92	0.68
1:C:65:ILE:HG22	1:C:66:PRO:N	2.09	0.68
1:C:98:TRP:HE3	1:C:102:THR:OG1	1.75	0.68
1:C:153:SER:HB3	4:C:2002:HOH:O	1.93	0.68
1:C:190:PRO:O	1:C:191:GLY:O	2.11	0.68
1:E:323:GLN:HA	1:E:330:TYR:CD1	2.29	0.68
1:A:282:ASP:OD1	1:A:282:ASP:N	2.27	0.68
1:A:357:LEU:HB3	1:A:358:TYR:CE1	2.27	0.68
1:C:220:VAL:HG21	1:C:249:ARG:CZ	2.23	0.68
1:C:225:LEU:HD23	1:C:228:PHE:CD2	2.29	0.68
1:C:252:VAL:HG13	1:C:253:PRO:HD2	1.76	0.68
1:F:63:GLY:O	1:F:66:PRO:HD2	1.93	0.68
1:C:426:ILE:HG22	1:C:437:GLY:CA	2.23	0.68
1:E:308:LYS:H	1:E:325:ASN:ND2	1.90	0.68
1:F:263:THR:CB	1:F:264:PRO:CD	2.71	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:PRO:HG2	1:B:453:ALA:CB	2.24	0.68
1:C:31:ALA:O	1:C:33:LYS:N	2.27	0.68
1:A:250:GLN:O	1:A:273:SER:HB2	1.94	0.67
1:B:91:GLU:O	1:B:93:THR:N	2.27	0.67
1:C:188:TYR:CE1	1:C:263:THR:O	2.48	0.67
1:A:461:THR:HG23	1:A:464:GLN:OE1	1.94	0.67
1:C:36:LYS:O	1:C:38:VAL:HG13	1.94	0.67
1:C:161:THR:O	2:C:600:FAD:H52A	1.93	0.67
1:F:422:TYR:HD1	1:F:422:TYR:C	1.97	0.67
1:B:291:VAL:CG2	3:B:601:NDP:C4A	2.73	0.67
1:E:275:ASN:O	1:E:276:SER:HB2	1.95	0.67
1:B:200:TYR:O	1:B:204:GLU:HG3	1.92	0.67
1:B:233:ALA:HA	1:B:236:ILE:HD12	1.76	0.67
1:B:238:GLU:O	1:B:242:GLU:HG3	1.95	0.67
1:A:318:VAL:HG12	1:A:319:THR:O	1.95	0.67
1:B:229:ASP:C	1:B:229:ASP:OD1	2.32	0.67
1:B:319:THR:HG23	1:B:323:GLN:O	1.95	0.67
1:F:49:LEU:HD22	1:F:49:LEU:N	2.09	0.67
1:B:250:GLN:O	1:B:273:SER:CB	2.43	0.67
1:C:188:TYR:O	1:C:190:PRO:HD3	1.94	0.67
1:D:38:VAL:HG23	1:D:125:VAL:HG13	1.77	0.67
1:D:167:TYR:HB3	1:D:173:ASP:OD2	1.95	0.67
1:F:150:LYS:HD3	1:F:152:TYR:OH	1.95	0.67
1:F:422:TYR:HE1	1:F:424:LYS:HB3	1.59	0.67
1:B:167:TYR:HB3	1:B:173:ASP:OD2	1.95	0.66
1:C:400:GLU:HA	1:C:400:GLU:OE1	1.94	0.66
1:E:473:PRO:O	1:E:473:PRO:HG2	1.94	0.66
1:F:428:ASN:HD22	1:F:431:ASP:HB2	1.59	0.66
1:A:114:TRP:HB3	1:D:114:TRP:HE1	1.59	0.66
1:A:378:LEU:CG	1:A:441:LEU:HD11	2.23	0.66
1:B:260:GLU:OE1	1:B:266:ARG:NH1	2.28	0.66
1:B:374:VAL:HG13	1:B:374:VAL:O	1.94	0.66
1:C:208:PHE:CD1	1:C:209:LEU:N	2.64	0.66
1:F:250:GLN:O	1:F:273:SER:HB3	1.94	0.66
1:D:480:THR:HG23	1:D:481:THR:HG23	1.76	0.66
1:F:380:TYR:OH	1:F:439:HIS:CD2	2.47	0.66
1:A:418:ASN:ND2	1:A:419:ASN:N	2.43	0.66
1:B:64:CYS:SG	2:B:600:FAD:C10	2.84	0.66
1:D:85:ASN:HB2	1:D:413:VAL:HG12	1.77	0.66
1:F:84:ARG:HH11	1:F:84:ARG:HB2	1.60	0.66
1:F:361:SER:HG	1:F:363:VAL:HG23	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:422:TYR:CD1	1:F:422:TYR:C	2.69	0.66
1:B:66:PRO:CG	1:B:109:ILE:HD11	2.26	0.66
1:E:98:TRP:CE2	1:E:102:THR:HG21	2.31	0.66
1:E:168:LEU:HD11	1:E:291:VAL:HG21	1.78	0.66
1:E:280:ILE:O	1:E:280:ILE:HG13	1.96	0.66
1:F:324:THR:OG1	1:F:329:ILE:O	2.10	0.66
1:C:208:PHE:HE1	1:C:209:LEU:HD22	1.55	0.66
1:D:411:TRP:C	1:D:414:PRO:HD2	2.15	0.66
1:C:159:ILE:HG12	1:C:330:TYR:O	1.95	0.66
1:C:325:ASN:H	1:C:325:ASN:HD22	1.41	0.66
1:A:313:THR:O	1:A:313:THR:OG1	2.11	0.66
1:B:144:ASN:OD1	1:B:145:ASN:N	2.29	0.66
1:A:192:LYS:H	1:A:285:ASN:HD22	1.44	0.65
1:E:281:GLU:O	1:E:282:ASP:C	2.34	0.65
1:C:310:ASN:OD1	1:C:313:THR:HG23	1.96	0.65
1:E:49:LEU:HD22	1:E:49:LEU:N	2.12	0.65
1:C:176:TYR:CE2	1:C:258:GLN:HB3	2.31	0.65
1:C:191:GLY:O	1:C:193:THR:HG22	1.96	0.65
1:D:220:VAL:HG21	1:D:249:ARG:HE	1.61	0.65
1:B:120:LEU:HD22	1:B:125:VAL:HG11	1.79	0.65
1:C:170:ILE:HB	1:C:254:THR:O	1.97	0.65
1:C:492:ILE:O	1:C:492:ILE:HG22	1.97	0.65
1:D:343:THR:HB	1:D:344:PRO:CD	2.27	0.65
1:F:223:ILE:CD1	1:F:230:GLN:NE2	2.60	0.65
1:B:91:GLU:OE1	1:B:92:ASP:N	2.30	0.65
1:B:399:ILE:HD12	1:B:427:CYS:O	1.96	0.65
1:F:428:ASN:HD22	1:F:431:ASP:HB3	1.60	0.65
1:A:68:LYS:HG2	1:B:409:LEU:HD23	1.77	0.65
1:B:65:ILE:HG22	1:B:66:PRO:CD	2.26	0.65
1:E:343:THR:CB	1:E:344:PRO:HD3	2.26	0.65
1:B:308:LYS:H	1:B:325:ASN:HD21	1.43	0.65
1:A:281:GLU:O	1:A:282:ASP:C	2.35	0.65
1:C:96:HIS:CE1	1:D:86:TYR:O	2.46	0.64
1:E:67:LYS:NZ	1:E:204:GLU:OE1	2.26	0.64
1:E:98:TRP:NE1	1:E:102:THR:HG21	2.12	0.64
1:E:423:ALA:HB3	1:E:478:ILE:HD13	1.79	0.64
1:A:373:THR:HG23	1:B:471:ILE:CG2	2.26	0.64
1:A:98:TRP:CD1	1:A:102:THR:HG21	2.31	0.64
1:A:291:VAL:CG1	3:A:601:NDP:C4A	2.75	0.64
1:B:263:THR:O	1:B:265:GLY:N	2.31	0.64
1:B:378:LEU:CD1	1:B:441:LEU:HG	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:VAL:HG13	3:C:601:NDP:N9A	2.12	0.64
1:D:262:GLY:O	1:D:263:THR:O	2.15	0.64
1:F:256:ILE:HD12	1:F:256:ILE:C	2.17	0.64
1:A:450:GLN:HE22	1:B:470:GLY:HA2	1.61	0.64
1:A:34:PHE:CE2	1:A:359:GLY:HA2	2.33	0.64
1:B:487:ARG:HG3	1:B:487:ARG:O	1.97	0.64
1:C:411:TRP:C	1:C:414:PRO:HD2	2.17	0.64
1:C:133:LYS:HD3	1:C:301:GLY:N	2.12	0.64
1:C:189:CYS:O	1:C:191:GLY:N	2.31	0.64
1:D:419:ASN:O	1:D:420:LYS:HD3	1.98	0.64
1:F:321:GLU:O	1:F:322:GLU:HB2	1.98	0.64
1:A:82:ASP:OD1	1:A:416:ARG:NH1	2.31	0.64
1:E:138:HIS:HD2	1:E:154:ALA:O	1.80	0.64
1:A:249:ARG:HB3	1:A:250:GLN:NE2	2.14	0.64
1:D:371:PRO:C	1:D:372:THR:HG22	2.18	0.64
1:F:22:SER:HB3	1:F:343:THR:HG23	1.80	0.64
1:B:55:LEU:HD13	1:B:116:TYR:HB3	1.80	0.63
1:C:323:GLN:HB2	1:C:330:TYR:CE2	2.33	0.63
1:F:230:GLN:O	1:F:234:ASN:ND2	2.31	0.63
1:F:489:GLY:O	1:F:490:GLY:C	2.34	0.63
1:E:186:LEU:HD22	1:E:188:TYR:CZ	2.34	0.63
1:C:374:VAL:O	1:C:374:VAL:HG12	1.97	0.63
1:E:38:VAL:CG2	1:E:125:VAL:HG13	2.27	0.63
1:E:72:GLN:HG3	1:E:76:LEU:HD22	1.80	0.63
1:E:98:TRP:O	1:E:102:THR:HG23	1.97	0.63
1:E:378:LEU:HD23	1:E:441:LEU:HD21	1.81	0.63
1:F:291:VAL:HG13	1:F:291:VAL:O	1.99	0.63
1:B:308:LYS:H	1:B:325:ASN:ND2	1.97	0.63
1:F:30:GLU:OE2	1:F:33:LYS:NZ	2.29	0.63
1:F:472:HIS:ND1	1:F:473:PRO:HA	2.12	0.63
1:C:343:THR:HB	1:C:344:PRO:HD3	1.78	0.63
1:F:167:TYR:HB3	1:F:173:ASP:OD2	1.99	0.63
1:C:161:THR:HG23	1:C:335:ILE:HD11	1.80	0.63
1:E:91:GLU:O	1:E:93:THR:N	2.31	0.63
1:F:217:THR:HG23	1:F:246:LYS:HB2	1.81	0.63
1:C:173:ASP:O	1:C:177:CYS:HB2	1.99	0.62
1:C:291:VAL:O	1:C:291:VAL:CG1	2.47	0.62
1:D:284:PHE:CD1	1:D:284:PHE:N	2.67	0.62
1:C:135:ILE:HG12	1:C:136:GLY:N	2.14	0.62
1:C:322:GLU:OE1	1:C:356:ARG:NH2	2.32	0.62
1:D:258:GLN:NE2	1:D:261:ALA:HB2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ILE:CG2	1:F:373:THR:HG23	2.28	0.62
1:F:84:ARG:HB2	1:F:84:ARG:NH1	2.13	0.62
1:B:110:GLY:HA2	1:B:113:ASN:HD22	1.64	0.62
1:B:204:GLU:OE2	1:B:375:PHE:N	2.26	0.62
1:D:418:ASN:HD22	1:D:419:ASN:N	1.97	0.62
1:D:177:CYS:SG	1:D:256:ILE:HD13	2.40	0.62
1:D:448:VAL:HG22	1:D:476:ALA:HB2	1.82	0.62
1:E:9:LYS:HG3	1:E:10:SER:N	2.15	0.62
1:F:108:HIS:O	1:F:111:SER:HB3	1.99	0.62
1:D:208:PHE:CE1	1:D:209:LEU:HD13	2.35	0.62
1:E:108:HIS:O	1:E:111:SER:HB3	2.00	0.62
1:E:434:ARG:HH11	1:E:434:ARG:CG	2.11	0.62
1:F:343:THR:HB	1:F:344:PRO:HD3	1.80	0.62
1:A:378:LEU:HD23	1:A:441:LEU:HD21	1.82	0.62
1:C:18:ILE:HG12	1:C:159:ILE:HA	1.80	0.62
1:C:47:THR:HB	1:C:48:PRO:HD2	1.81	0.62
1:C:176:TYR:CD2	1:C:258:GLN:HB3	2.35	0.62
1:C:234:ASN:HD22	1:C:234:ASN:N	1.97	0.62
1:F:70:MET:HG2	1:F:101:MET:HE3	1.82	0.62
1:F:98:TRP:O	1:F:102:THR:HG23	2.00	0.62
1:B:313:THR:O	1:B:313:THR:OG1	2.12	0.61
1:C:18:ILE:HD11	1:C:159:ILE:HG23	1.81	0.61
1:C:404:SER:HA	1:C:492:ILE:HG23	1.82	0.61
1:C:406:PHE:CZ	1:C:421:CYS:HB3	2.35	0.61
1:E:321:GLU:O	1:E:322:GLU:HB2	1.99	0.61
1:A:65:ILE:HG22	1:A:66:PRO:HD3	1.83	0.61
1:C:98:TRP:CD1	1:C:190:PRO:HD2	2.33	0.61
1:C:472:HIS:CD2	1:C:473:PRO:HA	2.35	0.61
1:D:222:SER:OG	3:D:601:NDP:O3X	2.15	0.61
1:F:281:GLU:O	1:F:282:ASP:C	2.36	0.61
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.13	0.61
1:E:58:THR:HG21	1:E:293:ARG:NH2	2.16	0.61
1:C:234:ASN:HD22	1:C:234:ASN:H	1.47	0.61
1:C:328:TYR:CD1	1:C:329:ILE:HG13	2.35	0.61
1:E:373:THR:HG21	1:E:446:GLY:HA2	1.82	0.61
1:F:262:GLY:O	1:F:263:THR:O	2.18	0.61
1:C:98:TRP:CD1	1:C:189:CYS:CA	2.69	0.61
1:C:193:THR:HB	1:C:286:THR:HB	1.82	0.61
1:E:411:TRP:C	1:E:414:PRO:HD2	2.21	0.61
1:B:250:GLN:O	1:B:273:SER:HB2	2.00	0.61
1:F:370:VAL:HG23	1:F:370:VAL:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLU:OE2	1:B:68:LYS:NZ	2.34	0.61
1:B:29:LYS:CG	1:B:30:GLU:N	2.64	0.61
1:A:411:TRP:C	1:A:414:PRO:HD2	2.21	0.61
1:B:59:CYS:HG	1:B:64:CYS:CB	2.13	0.61
1:B:431:ASP:O	1:B:432:ASN:HB2	2.00	0.61
1:A:478:ILE:N	1:A:478:ILE:CD1	2.54	0.61
1:B:13:PHE:O	1:B:154:ALA:HA	2.00	0.61
1:B:256:ILE:CD1	1:B:267:LEU:HB3	2.31	0.61
1:C:163:GLU:HB3	1:C:294:ASP:O	2.00	0.61
1:C:418:ASN:HD22	1:C:419:ASN:N	1.98	0.61
1:E:477:GLU:O	1:E:480:THR:HB	2.01	0.61
1:A:374:VAL:CG1	1:A:376:THR:HG23	2.30	0.60
1:B:221:ARG:HD2	1:B:252:VAL:HG21	1.82	0.60
1:D:323:GLN:HG3	1:D:330:TYR:CE1	2.36	0.60
1:F:163:GLU:HB3	1:F:295:SER:HA	1.83	0.60
1:C:72:GLN:NE2	1:D:410:GLU:HB3	2.03	0.60
1:C:427:CYS:HB3	1:C:433:GLU:O	2.01	0.60
1:E:322:GLU:HG2	1:E:332:ILE:CD1	2.31	0.60
1:F:62:VAL:HG23	1:F:62:VAL:O	2.01	0.60
1:F:431:ASP:OD1	1:F:434:ARG:NH1	2.34	0.60
1:A:144:ASN:CG	1:A:145:ASN:N	2.54	0.60
1:C:183:LEU:C	1:C:185:SER:H	2.05	0.60
1:C:55:LEU:HD13	1:C:116:TYR:HB3	1.82	0.60
1:C:68:LYS:O	1:C:71:HIS:HB3	2.01	0.60
1:C:398:ASN:OD1	1:C:430:LYS:HG3	2.00	0.60
1:D:323:GLN:HA	1:D:330:TYR:CD1	2.37	0.60
1:E:431:ASP:CG	1:E:434:ARG:NH1	2.54	0.60
1:F:461:THR:OG1	1:F:464:GLN:HG3	2.01	0.60
1:A:348:GLN:NE2	1:A:351:ARG:NH1	2.45	0.60
1:C:31:ALA:C	1:C:33:LYS:H	2.05	0.60
1:C:198:ALA:HB2	1:C:220:VAL:HG12	1.82	0.60
1:C:222:SER:OG	3:C:601:NDP:O3X	2.16	0.60
1:C:318:VAL:HG13	1:C:319:THR:N	2.15	0.60
1:C:405:PHE:H	1:C:492:ILE:HG22	1.66	0.60
1:D:321:GLU:O	1:D:322:GLU:HB2	1.99	0.60
1:B:291:VAL:O	1:B:291:VAL:HG13	2.01	0.60
1:C:275:ASN:O	1:C:276:SER:HB2	2.00	0.60
1:F:426:ILE:C	1:F:426:ILE:HD12	2.22	0.60
1:A:324:THR:OG1	1:A:329:ILE:O	2.18	0.60
1:A:440:VAL:HB	1:A:479:PHE:HZ	1.67	0.60
1:D:77:GLY:O	1:D:80:LEU:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:58:THR:OG1	2:E:600:FAD:O1A	2.19	0.60
1:E:72:GLN:HA	1:E:72:GLN:HE21	1.67	0.60
1:B:16:ILE:HB	1:B:157:PHE:CE1	2.37	0.60
1:B:263:THR:CB	1:B:264:PRO:CD	2.80	0.60
1:F:411:TRP:C	1:F:414:PRO:HD2	2.22	0.60
1:A:96:HIS:HE1	1:B:86:TYR:O	1.84	0.59
1:B:193:THR:CG2	1:B:286:THR:HB	2.28	0.59
1:B:492:ILE:C	1:B:493:LEU:HD23	2.22	0.59
3:B:601:NDP:O1A	3:B:601:NDP:H52N	2.02	0.59
1:C:36:LYS:HE3	1:C:358:TYR:HD2	1.67	0.59
1:C:223:ILE:O	1:C:223:ILE:HG13	2.02	0.59
1:C:336:LEU:HB3	1:C:339:LYS:HG3	1.84	0.59
1:D:236:ILE:HG13	1:D:441:LEU:HD11	1.83	0.59
1:A:373:THR:HG21	1:A:446:GLY:CA	2.32	0.59
1:F:30:GLU:O	1:F:31:ALA:C	2.39	0.59
1:F:263:THR:OG1	1:F:264:PRO:HD2	2.02	0.59
1:A:220:VAL:HG22	1:A:249:ARG:HA	1.84	0.59
1:C:47:THR:HB	1:C:48:PRO:CD	2.33	0.59
1:C:133:LYS:HD3	1:C:300:ILE:C	2.23	0.59
1:F:434:ARG:HE	1:F:461:THR:HG22	1.67	0.59
1:A:477:GLU:O	1:A:480:THR:HG22	2.03	0.59
1:C:58:THR:CB	2:C:600:FAD:O2A	2.51	0.59
1:C:302:LEU:HD21	1:C:309:ILE:HG12	1.85	0.59
1:E:30:GLU:O	1:E:31:ALA:C	2.40	0.59
1:E:221:ARG:NH1	3:E:601:NDP:O3X	2.36	0.59
1:F:173:ASP:OD1	1:F:174:LYS:N	2.34	0.59
1:F:203:LEU:HD12	1:F:225:LEU:HD21	1.84	0.59
1:D:473:PRO:O	1:D:473:PRO:CG	2.47	0.59
1:E:272:LYS:HG2	1:E:273:SER:N	2.17	0.59
1:F:55:LEU:HD13	1:F:116:TYR:HB3	1.83	0.59
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.85	0.59
1:C:255:LYS:O	1:C:255:LYS:HD3	2.02	0.59
1:E:266:ARG:C	1:E:267:LEU:HD13	2.22	0.59
1:A:65:ILE:CG2	1:A:66:PRO:HD3	2.33	0.59
1:B:167:TYR:CE2	1:B:174:LYS:HA	2.38	0.59
1:B:250:GLN:O	1:B:273:SER:HB3	2.02	0.59
1:C:263:THR:CB	1:C:264:PRO:HD3	2.32	0.59
1:C:438:PHE:HE2	1:C:452:PHE:CG	2.20	0.59
1:D:431:ASP:OD2	1:D:434:ARG:NH1	2.36	0.59
1:E:203:LEU:HD22	1:E:240:MET:CE	2.33	0.59
1:A:295:SER:CB	1:A:335:ILE:HD12	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LYS:HE3	1:D:276:SER:HA	1.84	0.59
1:D:281:GLU:O	1:D:282:ASP:C	2.39	0.59
1:E:418:ASN:ND2	1:E:419:ASN:H	1.99	0.59
1:A:114:TRP:CB	1:D:114:TRP:NE1	2.60	0.59
1:A:123:LYS:O	1:A:124:LYS:HB2	2.02	0.59
1:C:167:TYR:CE2	1:C:174:LYS:HA	2.38	0.59
1:F:336:LEU:HD23	1:F:339:LYS:HG3	1.85	0.59
1:C:167:TYR:HB3	1:C:173:ASP:OD2	2.03	0.58
1:C:183:LEU:O	1:C:185:SER:N	2.36	0.58
1:C:401:VAL:HG21	1:C:486:LYS:HD2	1.85	0.58
1:C:150:LYS:HD2	1:C:152:TYR:OH	2.03	0.58
1:C:325:ASN:H	1:C:325:ASN:ND2	2.00	0.58
1:C:328:TYR:CE1	1:C:329:ILE:HG13	2.38	0.58
1:A:357:LEU:C	1:A:358:TYR:HD1	2.07	0.58
1:B:356:ARG:HH11	1:B:364:LYS:HA	1.67	0.58
1:C:22:SER:HB3	1:C:343:THR:HG23	1.85	0.58
1:C:441:LEU:HD12	1:C:441:LEU:C	2.23	0.58
1:D:158:LEU:HD11	1:D:332:ILE:HB	1.85	0.58
1:D:220:VAL:HG21	1:D:249:ARG:NE	2.17	0.58
1:F:263:THR:HB	1:F:264:PRO:CD	2.32	0.58
1:A:240:MET:HE2	1:A:247:PHE:HZ	1.69	0.58
1:B:200:TYR:HB2	1:B:374:VAL:HG23	1.85	0.58
1:D:413:VAL:N	1:D:414:PRO:CD	2.66	0.58
1:E:322:GLU:HG2	1:E:332:ILE:HD12	1.85	0.58
1:F:203:LEU:HD12	1:F:225:LEU:CD2	2.33	0.58
1:B:426:ILE:HG12	1:B:437:GLY:CA	2.31	0.58
1:C:285:ASN:H	1:C:285:ASN:ND2	1.98	0.58
1:D:162:GLY:O	1:D:335:ILE:HD11	2.03	0.58
1:F:168:LEU:HB3	1:F:170:ILE:CG2	2.24	0.58
1:F:315:LYS:HE3	1:F:336:LEU:O	2.04	0.58
1:D:52:ASN:N	1:D:52:ASN:ND2	2.49	0.58
1:D:98:TRP:O	1:D:102:THR:HG23	2.03	0.58
1:D:402:TYR:OH	1:D:433:GLU:OE1	2.19	0.58
1:E:158:LEU:HD11	1:E:332:ILE:HB	1.85	0.58
1:A:158:LEU:HD11	1:A:332:ILE:HG13	1.84	0.58
1:C:208:PHE:O	1:C:209:LEU:C	2.42	0.58
1:D:251:PHE:CD1	1:D:273:SER:CB	2.82	0.58
1:D:263:THR:HB	1:D:264:PRO:HD3	1.86	0.58
1:E:40:VAL:HG22	1:E:40:VAL:O	2.03	0.58
1:F:67:LYS:HE2	2:F:600:FAD:H6	1.86	0.58
1:F:193:THR:HB	1:F:286:THR:HB	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:GLU:O	1:A:31:ALA:C	2.41	0.58
1:A:250:GLN:O	1:A:251:PHE:CD1	2.57	0.58
1:A:358:TYR:N	1:A:358:TYR:HD1	2.02	0.58
1:B:22:SER:OG	1:B:343:THR:HG23	2.03	0.58
1:C:342:LEU:HB2	1:C:345:VAL:CG2	2.33	0.58
1:E:223:ILE:HD11	1:E:230:GLN:HG3	1.84	0.58
1:F:380:TYR:CD1	1:F:380:TYR:C	2.72	0.58
1:B:387:GLU:OE1	1:B:424:LYS:NZ	2.33	0.58
1:C:473:PRO:O	1:C:473:PRO:HG2	2.04	0.58
1:D:425:VAL:HG13	1:D:435:VAL:HG13	1.86	0.58
1:F:318:VAL:CG2	1:F:322:GLU:C	2.73	0.58
1:B:394:PHE:CE2	1:B:428:ASN:ND2	2.72	0.57
1:B:431:ASP:OD2	1:B:434:ARG:NH1	2.37	0.57
1:C:318:VAL:CG1	1:C:319:THR:O	2.52	0.57
1:F:321:GLU:HG2	1:F:356:ARG:HH11	1.69	0.57
1:E:336:LEU:HB3	1:E:339:LYS:CG	2.34	0.57
1:F:232:MET:O	1:F:236:ILE:HG13	2.04	0.57
1:B:131:TYR:CE1	2:B:600:FAD:N6A	2.71	0.57
1:C:168:LEU:HD23	1:C:170:ILE:HD13	1.86	0.57
1:D:63:GLY:O	1:D:66:PRO:HD2	2.04	0.57
1:B:263:THR:OG1	1:B:264:PRO:HD2	2.04	0.57
1:E:410:GLU:HG2	1:F:72:GLN:NE2	2.19	0.57
1:F:186:LEU:HD12	1:F:188:TYR:O	2.04	0.57
1:A:406:PHE:CZ	1:A:421:CYS:HB3	2.39	0.57
1:F:97:ASP:C	1:F:97:ASP:OD1	2.43	0.57
1:F:323:GLN:HG3	1:F:330:TYR:CE1	2.39	0.57
1:A:189:CYS:SG	1:A:190:PRO:HD2	2.45	0.57
1:A:205:CYS:HA	1:A:208:PHE:CE2	2.40	0.57
1:E:410:GLU:CG	1:F:72:GLN:NE2	2.67	0.57
1:F:396:GLU:C	1:F:396:GLU:CD	2.62	0.57
1:F:400:GLU:OE1	1:F:487:ARG:NH1	2.38	0.57
1:B:368:ASP:O	1:B:369:ASN:HB2	2.05	0.57
1:D:178:ILE:HB	1:D:182:ASP:HB2	1.85	0.57
1:D:325:ASN:N	1:D:325:ASN:ND2	2.34	0.57
1:C:225:LEU:HB3	1:C:228:PHE:HB2	1.86	0.57
1:F:39:MET:HE3	1:F:41:LEU:HD21	1.87	0.57
1:A:76:LEU:O	1:A:79:ALA:HB3	2.05	0.56
1:A:418:ASN:HD22	1:A:419:ASN:N	1.99	0.56
1:C:178:ILE:HB	1:C:182:ASP:HB2	1.86	0.56
1:C:223:ILE:O	1:C:223:ILE:CG1	2.52	0.56
1:D:30:GLU:O	1:D:33:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LEU:HD21	1:B:90:LEU:CD2	2.35	0.56
1:A:220:VAL:HG21	1:A:249:ARG:NE	2.17	0.56
1:C:195:VAL:HB	1:C:218:VAL:HG22	1.87	0.56
1:D:426:ILE:HD12	1:D:427:CYS:N	2.20	0.56
1:F:258:GLN:HE22	1:F:261:ALA:HB2	1.69	0.56
1:F:440:VAL:O	1:F:440:VAL:HG13	2.04	0.56
1:C:137:PRO:O	1:C:138:HIS:HB2	2.05	0.56
1:D:62:VAL:O	1:D:62:VAL:HG23	2.04	0.56
1:E:411:TRP:O	1:E:414:PRO:HD2	2.06	0.56
1:E:471:ILE:HG21	1:F:373:THR:CG2	2.34	0.56
1:F:82:ASP:OD1	1:F:416:ARG:NH1	2.38	0.56
1:F:168:LEU:HD23	1:F:170:ILE:HD13	1.87	0.56
1:B:25:LEU:HD13	1:B:116:TYR:CD1	2.41	0.56
1:B:173:ASP:OD1	1:B:174:LYS:N	2.34	0.56
1:B:403:HIS:NE2	1:B:492:ILE:HD13	2.21	0.56
1:C:194:LEU:HD23	1:C:194:LEU:C	2.25	0.56
1:C:493:LEU:HD12	1:C:493:LEU:N	2.19	0.56
1:D:108:HIS:CE1	1:D:112:LEU:HD11	2.40	0.56
1:F:34:PHE:HZ	1:F:355:GLN:NE2	2.03	0.56
1:A:188:TYR:CD2	1:A:263:THR:HB	2.40	0.56
1:B:65:ILE:CB	1:B:66:PRO:CD	2.82	0.56
1:B:325:ASN:ND2	1:B:325:ASN:H	2.03	0.56
1:D:91:GLU:O	1:D:93:THR:N	2.39	0.56
1:D:250:GLN:O	1:D:251:PHE:CD1	2.59	0.56
1:C:172:GLY:CA	1:C:175:GLU:HG3	2.24	0.56
1:D:434:ARG:HG2	1:D:434:ARG:HH11	1.71	0.56
1:E:170:ILE:HD11	1:E:253:PRO:HB2	1.86	0.56
1:F:291:VAL:O	1:F:291:VAL:CG1	2.53	0.56
1:D:83:SER:HB2	1:D:88:TRP:HB2	1.87	0.56
1:E:215:ASP:C	1:E:215:ASP:OD1	2.44	0.56
1:F:96:HIS:CD2	1:F:212:ILE:HG13	2.41	0.56
1:B:263:THR:HB	1:B:264:PRO:HD3	1.88	0.56
1:B:239:HIS:CE1	1:B:378:LEU:HB2	2.41	0.56
1:D:51:THR:C	1:D:52:ASN:ND2	2.59	0.56
1:E:373:THR:HG23	1:F:471:ILE:CG2	2.36	0.56
1:F:221:ARG:HH11	1:F:221:ARG:CG	2.19	0.56
1:A:343:THR:HB	1:A:344:PRO:HD3	1.88	0.55
1:B:70:MET:SD	1:B:101:MET:CE	2.94	0.55
1:B:321:GLU:O	1:B:322:GLU:HB2	2.04	0.55
1:C:200:TYR:O	1:C:204:GLU:HB2	2.06	0.55
1:C:259:ILE:HG23	1:C:259:ILE:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:GLU:HG3	1:C:356:ARG:NH1	2.21	0.55
1:D:316:ILE:HG13	1:D:335:ILE:HG22	1.88	0.55
1:F:474:VAL:O	1:F:477:GLU:HG2	2.06	0.55
1:B:199:SER:HA	1:B:225:LEU:HD23	1.88	0.55
1:D:406:PHE:CZ	1:D:421:CYS:HB3	2.41	0.55
1:E:267:LEU:HD13	1:E:267:LEU:N	2.21	0.55
1:C:133:LYS:C	1:C:140:ILE:HG13	2.26	0.55
1:D:163:GLU:OE2	1:D:334:ASP:HB3	2.07	0.55
1:E:38:VAL:HG23	1:E:125:VAL:HG13	1.87	0.55
1:A:400:GLU:OE1	1:A:400:GLU:HA	2.06	0.55
1:A:401:VAL:O	1:A:401:VAL:HG12	2.07	0.55
1:C:15:LEU:HD12	1:C:156:ARG:O	2.07	0.55
1:A:47:THR:HG21	1:A:51:THR:OG1	2.07	0.55
1:C:66:PRO:HG3	1:C:109:ILE:HD11	1.88	0.55
1:D:324:THR:HG23	1:D:329:ILE:O	2.07	0.55
1:E:256:ILE:CD1	1:E:269:VAL:HG22	2.28	0.55
1:A:173:ASP:O	1:A:177:CYS:HB2	2.06	0.55
1:C:340:LEU:HG	1:C:370:VAL:HG21	1.88	0.55
1:D:175:GLU:OE1	1:D:175:GLU:N	2.39	0.55
1:F:158:LEU:HD12	1:F:159:ILE:N	2.22	0.55
1:A:108:HIS:O	1:A:111:SER:HB3	2.06	0.55
1:B:65:ILE:HB	1:B:66:PRO:CD	2.37	0.55
1:B:192:LYS:H	1:B:285:ASN:ND2	2.01	0.55
1:C:310:ASN:HD22	1:C:311:GLU:N	2.04	0.55
1:D:67:LYS:HD3	1:D:204:GLU:OE1	2.05	0.55
1:D:114:TRP:CZ3	1:D:118:VAL:CG2	2.90	0.55
1:D:407:TRP:CD1	1:D:418:ASN:HA	2.41	0.55
1:E:373:THR:HG23	1:F:471:ILE:HG21	1.89	0.55
1:C:21:GLY:HA2	1:C:57:GLY:HA3	1.88	0.55
1:D:194:LEU:HB2	1:D:284:PHE:CE2	2.42	0.55
1:E:141:MET:CE	1:E:149:GLU:OE2	2.55	0.55
1:E:497:CYS:SG	1:F:116:TYR:CD2	2.98	0.55
1:A:168:LEU:O	1:A:173:ASP:OD2	2.25	0.55
1:F:428:ASN:ND2	1:F:431:ASP:HB2	2.21	0.55
1:A:447:GLU:CD	1:B:474:VAL:HG13	2.28	0.54
1:B:419:ASN:O	1:B:420:LYS:HD3	2.07	0.54
1:B:461:THR:OG1	1:B:464:GLN:HG3	2.07	0.54
1:E:192:LYS:N	1:E:285:ASN:HD22	2.02	0.54
1:C:72:GLN:HE21	1:D:410:GLU:CB	2.05	0.54
1:C:319:THR:C	1:C:321:GLU:H	2.08	0.54
1:D:221:ARG:NH1	3:D:601:NDP:P2B	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:61:ASN:HA	1:E:109:ILE:HD13	1.88	0.54
1:F:68:LYS:HE2	1:F:375:PHE:CE2	2.43	0.54
1:F:343:THR:O	1:F:347:ILE:HG23	2.07	0.54
1:A:65:ILE:CB	1:A:66:PRO:HD3	2.37	0.54
1:A:196:VAL:O	1:A:291:VAL:HG22	2.07	0.54
1:C:47:THR:CB	1:C:48:PRO:CD	2.85	0.54
1:C:190:PRO:O	1:C:191:GLY:C	2.46	0.54
1:F:60:VAL:HG13	1:F:112:LEU:HD13	1.89	0.54
1:F:318:VAL:HG21	1:F:322:GLU:C	2.28	0.54
1:C:308:LYS:H	1:C:325:ASN:ND2	2.06	0.54
1:C:309:ILE:O	1:C:309:ILE:HG13	2.07	0.54
1:E:38:VAL:HG22	1:E:125:VAL:HG22	1.89	0.54
1:E:70:MET:HG2	1:E:101:MET:CE	2.38	0.54
1:E:185:SER:O	1:E:186:LEU:C	2.43	0.54
1:E:272:LYS:CE	1:E:276:SER:HA	2.37	0.54
1:F:13:PHE:O	1:F:154:ALA:HA	2.08	0.54
1:F:277:GLU:OE1	1:F:277:GLU:HA	2.07	0.54
1:A:98:TRP:CD1	1:A:102:THR:CG2	2.90	0.54
1:A:272:LYS:CE	1:A:276:SER:HA	2.36	0.54
1:B:402:TYR:CE2	1:B:462:LYS:HE3	2.41	0.54
1:C:343:THR:N	2:C:600:FAD:HO3'	2.06	0.54
1:F:221:ARG:NH1	3:F:601:NDP:O3X	2.41	0.54
1:A:12:ASP:HB2	1:A:153:SER:O	2.08	0.54
1:B:123:LYS:O	1:B:124:LYS:HB2	2.07	0.54
1:C:193:THR:OG1	1:C:194:LEU:N	2.39	0.54
1:E:232:MET:CE	1:E:441:LEU:HB2	2.34	0.54
1:E:305:VAL:O	1:E:305:VAL:HG12	2.08	0.54
1:C:286:THR:O	1:C:286:THR:HG22	2.07	0.54
1:C:370:VAL:HG23	1:C:370:VAL:O	2.07	0.54
1:D:236:ILE:CG1	1:D:441:LEU:HD11	2.38	0.54
1:D:343:THR:CB	1:D:344:PRO:CD	2.84	0.54
1:D:426:ILE:HD12	1:D:426:ILE:C	2.29	0.54
1:E:383:CYS:SG	1:E:456:LEU:HD12	2.48	0.54
1:A:98:TRP:HE1	1:A:102:THR:HG21	1.70	0.54
1:D:418:ASN:ND2	1:D:419:ASN:N	2.56	0.54
1:E:426:ILE:O	1:E:426:ILE:HG13	2.07	0.54
1:A:90:LEU:CD2	1:B:90:LEU:HD21	2.36	0.53
1:A:177:CYS:SG	1:A:256:ILE:HD12	2.47	0.53
1:B:332:ILE:HG12	1:B:333:GLY:N	2.23	0.53
1:D:78:GLN:NE2	1:D:82:ASP:OD1	2.41	0.53
1:F:192:LYS:N	1:F:285:ASN:ND2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:GLY:O	1:A:193:THR:CG2	2.56	0.53
1:A:313:THR:O	1:A:315:LYS:N	2.42	0.53
1:B:172:GLY:HA2	1:B:175:GLU:CG	2.37	0.53
1:B:222:SER:OG	3:B:601:NDP:O3X	2.24	0.53
1:C:376:THR:HB	1:C:377:PRO:CD	2.39	0.53
1:E:141:MET:HE1	1:E:149:GLU:OE2	2.09	0.53
1:B:472:HIS:ND1	1:B:473:PRO:HA	2.23	0.53
1:D:98:TRP:CE2	1:D:102:THR:HG21	2.43	0.53
1:D:478:ILE:HD12	1:D:478:ILE:N	2.24	0.53
1:F:470:GLY:HA2	1:F:480:THR:HG21	1.89	0.53
1:B:131:TYR:CE2	2:B:600:FAD:N6A	2.77	0.53
1:C:432:ASN:O	1:C:433:GLU:HB2	2.08	0.53
1:D:144:ASN:HD22	1:D:146:LYS:N	1.99	0.53
1:E:323:GLN:HB2	1:E:330:TYR:HE1	1.74	0.53
1:A:99:GLU:CG	1:D:146:LYS:HD3	2.35	0.53
1:A:240:MET:HE2	1:A:247:PHE:CZ	2.43	0.53
1:A:478:ILE:H	1:A:478:ILE:CD1	2.04	0.53
1:C:34:PHE:N	1:C:34:PHE:CD1	2.75	0.53
1:C:447:GLU:CD	1:D:474:VAL:HG13	2.29	0.53
1:D:66:PRO:HG3	1:D:109:ILE:HD11	1.91	0.53
1:D:221:ARG:HH12	3:D:601:NDP:P2B	2.31	0.53
1:D:263:THR:CB	1:D:264:PRO:HD3	2.39	0.53
1:E:431:ASP:OD1	1:E:431:ASP:O	2.25	0.53
1:F:318:VAL:HG23	1:F:323:GLN:O	2.09	0.53
1:B:281:GLU:O	1:B:282:ASP:O	2.26	0.53
1:C:103:GLU:O	1:C:107:ASN:HB2	2.08	0.53
1:D:272:LYS:CG	1:D:273:SER:N	2.70	0.53
1:F:438:PHE:CE1	1:F:479:PHE:CE1	2.96	0.53
1:A:249:ARG:HB3	1:A:250:GLN:HE22	1.73	0.53
1:C:58:THR:HB	2:C:600:FAD:O2A	2.09	0.53
1:C:376:THR:HB	1:C:377:PRO:HD2	1.90	0.53
1:F:194:LEU:HB2	1:F:284:PHE:CE2	2.44	0.53
1:A:163:GLU:HB3	1:A:295:SER:HA	1.91	0.53
1:C:310:ASN:HD22	1:C:310:ASN:C	2.12	0.53
1:C:421:CYS:HA	1:C:441:LEU:O	2.09	0.53
1:E:336:LEU:HB3	1:E:339:LYS:HG2	1.91	0.53
1:E:414:PRO:O	1:E:415:SER:HB2	2.09	0.53
1:B:263:THR:OG1	1:B:264:PRO:CD	2.57	0.52
1:C:283:GLU:H	1:C:283:GLU:CD	2.12	0.52
1:C:404:SER:HA	1:C:492:ILE:HG21	1.89	0.52
1:F:22:SER:CB	1:F:343:THR:HG23	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:LEU:HD21	1:F:249:ARG:NH1	2.24	0.52
1:A:471:ILE:CG2	1:B:373:THR:HG23	2.39	0.52
1:B:371:PRO:CG	1:B:453:ALA:HB1	2.37	0.52
1:C:356:ARG:HG2	1:C:361:SER:O	2.07	0.52
1:D:144:ASN:HB2	1:D:148:LYS:O	2.09	0.52
1:E:321:GLU:O	1:E:356:ARG:NH1	2.40	0.52
1:F:263:THR:O	1:F:265:GLY:N	2.42	0.52
1:A:98:TRP:NE1	1:A:102:THR:CG2	2.63	0.52
1:C:178:ILE:HD11	1:C:286:THR:HG22	1.90	0.52
1:C:221:ARG:O	1:C:250:GLN:HA	2.09	0.52
1:D:13:PHE:O	1:D:154:ALA:HA	2.09	0.52
1:F:267:LEU:O	1:F:283:GLU:HA	2.10	0.52
1:A:220:VAL:O	1:A:220:VAL:HG23	2.08	0.52
1:A:273:SER:OG	1:A:275:ASN:HB3	2.09	0.52
1:A:411:TRP:O	1:A:414:PRO:HD2	2.09	0.52
1:B:29:LYS:HG2	1:B:30:GLU:N	2.24	0.52
1:C:291:VAL:HG13	3:C:601:NDP:C4A	2.39	0.52
1:A:321:GLU:O	1:A:322:GLU:HB2	2.09	0.52
1:A:424:LYS:HG2	1:A:439:HIS:HB2	1.91	0.52
1:C:60:VAL:O	1:C:109:ILE:HD13	2.08	0.52
1:E:205:CYS:HA	1:E:208:PHE:CE2	2.44	0.52
1:F:110:GLY:HA2	1:F:113:ASN:ND2	2.22	0.52
1:F:258:GLN:NE2	1:F:261:ALA:N	2.58	0.52
1:A:200:TYR:O	1:A:204:GLU:HG3	2.09	0.52
1:A:450:GLN:HE22	1:B:471:ILE:H	1.58	0.52
3:A:601:NDP:O2N	3:A:601:NDP:O5B	2.27	0.52
1:C:114:TRP:CE3	1:C:117:ARG:HD2	2.45	0.52
1:D:272:LYS:NZ	1:D:276:SER:HA	2.25	0.52
1:E:186:LEU:CD2	1:E:188:TYR:CZ	2.93	0.52
1:E:273:SER:CB	1:E:275:ASN:OD1	2.58	0.52
1:B:55:LEU:HD13	1:B:116:TYR:CB	2.40	0.52
1:B:277:GLU:HG2	1:B:278:GLU:N	2.25	0.52
1:C:71:HIS:O	1:C:74:ALA:HB3	2.10	0.52
1:D:250:GLN:O	1:D:273:SER:HB3	2.07	0.52
1:F:167:TYR:CE2	1:F:174:LYS:HA	2.45	0.52
1:B:319:THR:CG2	1:B:323:GLN:HB3	2.39	0.52
1:B:488:SER:OG	1:B:489:GLY:N	2.43	0.52
1:C:116:TYR:O	1:C:119:ALA:HB3	2.10	0.52
1:C:224:LEU:HD11	1:C:249:ARG:HH12	1.75	0.52
1:C:366:ASP:C	1:C:366:ASP:OD1	2.48	0.52
1:D:343:THR:HB	1:D:344:PRO:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:LYS:HD2	1:A:68:LYS:N	2.24	0.52
1:A:193:THR:HB	1:A:286:THR:O	2.10	0.52
1:E:373:THR:HB	1:E:381:GLY:HA2	1.91	0.52
1:F:141:MET:CE	1:F:143:THR:OG1	2.58	0.52
1:F:336:LEU:HB3	1:F:339:LYS:HG2	1.92	0.52
1:A:82:ASP:OD2	1:A:416:ARG:NH1	2.40	0.52
1:B:91:GLU:OE1	1:B:91:GLU:C	2.48	0.52
1:C:114:TRP:O	1:C:118:VAL:HG23	2.10	0.52
1:D:317:PRO:C	1:D:318:VAL:HG13	2.31	0.52
1:D:336:LEU:HB3	1:D:339:LYS:CG	2.40	0.52
1:E:172:GLY:HA2	1:E:175:GLU:HG2	1.92	0.52
1:B:380:TYR:OH	1:B:439:HIS:HD2	1.93	0.51
1:C:308:LYS:H	1:C:325:ASN:HD21	1.58	0.51
1:C:348:GLN:O	1:C:352:LEU:HB2	2.10	0.51
1:D:407:TRP:CD2	1:D:418:ASN:CG	2.83	0.51
1:A:310:ASN:HD22	1:A:312:LYS:H	1.58	0.51
1:B:61:ASN:HA	1:B:109:ILE:HD13	1.91	0.51
1:C:138:HIS:HD2	1:C:328:TYR:CE2	2.29	0.51
1:D:336:LEU:HB3	1:D:339:LYS:HG2	1.93	0.51
1:E:108:HIS:NE2	1:F:412:THR:HG21	2.25	0.51
1:E:203:LEU:HD22	1:E:240:MET:SD	2.50	0.51
1:A:29:LYS:HG3	1:A:30:GLU:N	2.24	0.51
1:A:440:VAL:HB	1:A:479:PHE:CZ	2.45	0.51
1:B:440:VAL:HG13	1:B:440:VAL:O	2.09	0.51
1:C:168:LEU:HB3	1:C:170:ILE:HG23	1.92	0.51
1:C:403:HIS:CE1	1:C:492:ILE:CD1	2.87	0.51
1:E:343:THR:HB	1:E:344:PRO:CD	2.35	0.51
1:E:450:GLN:NE2	1:F:470:GLY:HA2	2.23	0.51
1:F:469:ILE:N	1:F:469:ILE:CD1	2.67	0.51
1:C:161:THR:HG23	1:C:335:ILE:HD13	1.92	0.51
1:C:285:ASN:N	1:C:285:ASN:ND2	2.54	0.51
1:D:272:LYS:CE	1:D:276:SER:HA	2.41	0.51
1:D:402:TYR:CD2	1:D:462:LYS:HE2	2.45	0.51
1:E:343:THR:CB	1:E:344:PRO:CD	2.89	0.51
1:A:474:VAL:HG13	1:B:447:GLU:CD	2.31	0.51
1:C:20:GLY:HA2	1:C:25:LEU:HD21	1.92	0.51
1:C:212:ILE:CG2	1:C:212:ILE:O	2.58	0.51
1:E:161:THR:HB	2:E:600:FAD:C8A	2.41	0.51
1:E:208:PHE:CE1	1:E:209:LEU:HD13	2.46	0.51
1:F:332:ILE:HG23	1:F:333:GLY:N	2.25	0.51
1:A:402:TYR:CD2	1:A:485:THR:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:TRP:O	1:C:102:THR:OG1	2.28	0.51
1:C:361:SER:OG	1:C:363:VAL:HG22	2.11	0.51
1:C:478:ILE:HD12	1:C:479:PHE:H	1.76	0.51
1:D:405:PHE:CD1	1:D:492:ILE:HD12	2.45	0.51
1:A:131:TYR:CE1	2:A:600:FAD:N6A	2.79	0.51
1:A:310:ASN:C	1:A:310:ASN:ND2	2.64	0.51
1:A:345:VAL:HG22	1:B:469:ILE:HD13	1.91	0.51
1:B:305:VAL:CG1	1:B:328:TYR:OH	2.59	0.51
1:B:409:LEU:O	1:B:412:THR:HG23	2.10	0.51
1:C:251:PHE:HE2	1:C:279:THR:HG1	1.59	0.51
1:C:260:GLU:HB2	1:C:266:ARG:HB3	1.93	0.51
1:A:380:TYR:OH	1:A:439:HIS:HD2	1.93	0.51
1:C:86:TYR:O	1:D:101:MET:HB2	2.10	0.51
1:C:405:PHE:H	1:C:492:ILE:CG2	2.22	0.51
1:C:412:THR:O	1:C:415:SER:N	2.40	0.51
1:D:291:VAL:HG22	3:D:601:NDP:C4A	2.41	0.51
1:F:434:ARG:HG2	1:F:434:ARG:NH1	2.20	0.51
1:A:229:ASP:C	1:A:229:ASP:OD1	2.49	0.51
1:A:308:LYS:N	1:A:325:ASN:HD21	2.03	0.51
1:A:318:VAL:HG13	1:A:322:GLU:HA	1.89	0.51
1:B:328:TYR:HD1	1:B:328:TYR:H	1.59	0.51
1:D:376:THR:HB	1:D:377:PRO:CD	2.41	0.51
1:E:68:LYS:O	1:E:71:HIS:HB3	2.11	0.51
1:F:281:GLU:OE1	1:F:281:GLU:HA	2.10	0.51
1:A:96:HIS:CD2	1:A:212:ILE:HG23	2.46	0.51
1:A:236:ILE:HD11	1:A:380:TYR:CD2	2.45	0.51
1:A:428:ASN:ND2	1:A:431:ASP:CB	2.74	0.51
1:B:67:LYS:HE2	1:B:204:GLU:OE2	2.10	0.51
1:B:281:GLU:C	1:B:282:ASP:O	2.49	0.51
1:C:67:LYS:HE2	2:C:600:FAD:H6	1.92	0.51
1:C:448:VAL:HG12	1:D:447:GLU:HB3	1.92	0.51
1:E:438:PHE:CZ	1:E:452:PHE:CD2	2.98	0.51
1:F:275:ASN:OD1	1:F:277:GLU:HG2	2.11	0.51
1:A:480:THR:HG23	1:A:481:THR:HG23	1.93	0.50
1:B:68:LYS:HE2	1:B:375:PHE:CE2	2.46	0.50
1:B:70:MET:SD	1:B:101:MET:HE3	2.51	0.50
1:B:402:TYR:HB3	1:B:482:LEU:HB3	1.93	0.50
1:D:478:ILE:HD12	1:D:479:PHE:N	2.26	0.50
1:E:140:ILE:HG23	1:E:140:ILE:O	2.10	0.50
1:E:426:ILE:HG12	1:E:437:GLY:CA	2.38	0.50
1:F:58:THR:HG22	1:F:62:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:NZ	2:B:600:FAD:O4	2.44	0.50
1:B:258:GLN:NE2	1:B:261:ALA:HB2	2.26	0.50
1:B:326:VAL:CG1	1:B:328:TYR:CE1	2.95	0.50
1:C:106:GLN:HA	1:C:109:ILE:HG13	1.93	0.50
1:C:220:VAL:HG21	1:C:249:ARG:CD	2.40	0.50
1:C:250:GLN:O	1:C:273:SER:HB2	2.11	0.50
1:C:449:THR:O	1:C:450:GLN:C	2.49	0.50
1:D:317:PRO:O	1:D:318:VAL:HG12	2.11	0.50
1:F:309:ILE:O	1:F:309:ILE:HG13	2.10	0.50
1:A:320:ASP:OD1	1:A:320:ASP:C	2.50	0.50
1:A:357:LEU:C	1:A:358:TYR:CD1	2.85	0.50
2:A:600:FAD:O2A	2:A:600:FAD:O5'	2.27	0.50
1:C:55:LEU:HD22	1:C:56:GLY:N	2.26	0.50
1:C:223:ILE:HD12	1:C:230:GLN:NE2	2.26	0.50
1:F:273:SER:OG	1:F:275:ASN:HB3	2.12	0.50
1:C:66:PRO:O	1:C:70:MET:HB2	2.12	0.50
1:D:411:TRP:CE2	1:D:416:ARG:NH2	2.80	0.50
1:E:487:ARG:O	1:E:487:ARG:HG3	2.11	0.50
1:F:58:THR:OG1	2:F:600:FAD:O1A	2.29	0.50
1:F:348:GLN:HG2	1:F:351:ARG:NH1	2.27	0.50
1:A:268:LYS:HE2	1:A:280:ILE:HD12	1.93	0.50
1:B:168:LEU:HD13	1:B:168:LEU:N	2.27	0.50
1:B:256:ILE:O	1:B:256:ILE:HG13	2.12	0.50
1:C:58:THR:OG1	2:C:600:FAD:O2A	2.30	0.50
1:C:80:LEU:O	1:C:81:LYS:C	2.50	0.50
1:C:266:ARG:HG3	1:C:283:GLU:HB3	1.94	0.50
2:C:600:FAD:O1A	2:C:600:FAD:H5'1	2.12	0.50
1:A:387:GLU:OE2	1:A:486:LYS:NZ	2.42	0.50
1:A:438:PHE:CE2	1:A:452:PHE:CG	3.00	0.50
1:C:75:LEU:O	1:C:78:GLN:N	2.43	0.50
1:C:133:LYS:HA	1:C:301:GLY:H	1.77	0.50
1:C:252:VAL:CG1	1:C:253:PRO:HD2	2.42	0.50
1:C:387:GLU:HA	1:C:426:ILE:HD13	1.93	0.50
1:D:193:THR:HG23	1:D:286:THR:O	2.12	0.50
1:E:34:PHE:CE2	1:E:359:GLY:HA2	2.46	0.50
1:E:71:HIS:CD2	1:E:375:PHE:HB3	2.46	0.50
1:E:170:ILE:CD1	1:E:253:PRO:HB2	2.41	0.50
1:A:62:VAL:HG23	1:A:62:VAL:O	2.11	0.50
1:A:91:GLU:O	1:A:93:THR:N	2.45	0.50
1:A:204:GLU:OE2	1:A:375:PHE:N	2.40	0.50
1:C:75:LEU:O	1:C:76:LEU:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:CYS:C	1:C:191:GLY:H	2.15	0.50
1:C:220:VAL:CG2	1:C:249:ARG:HD2	2.41	0.50
1:C:228:PHE:O	1:C:229:ASP:C	2.48	0.50
1:C:365:CYS:SG	1:C:367:TYR:CZ	3.05	0.50
1:D:170:ILE:O	1:D:170:ILE:HG13	2.12	0.50
1:B:168:LEU:O	1:B:173:ASP:OD2	2.30	0.50
1:B:318:VAL:HG22	1:B:323:GLN:O	2.11	0.50
1:D:167:TYR:CE2	1:D:174:LYS:HA	2.46	0.50
1:E:195:VAL:HG21	1:E:206:ALA:HB2	1.93	0.50
1:F:34:PHE:HZ	1:F:355:GLN:HE22	1.58	0.50
1:B:172:GLY:O	1:B:175:GLU:HG2	2.12	0.50
1:C:164:ARG:HB3	1:C:165:PRO:CD	2.36	0.50
1:F:172:GLY:HA2	1:F:175:GLU:CG	2.41	0.50
1:F:209:LEU:HG	1:F:214:LEU:HD12	1.94	0.50
1:F:434:ARG:HH11	1:F:434:ARG:CG	2.18	0.50
1:B:216:VAL:HG12	1:B:217:THR:N	2.26	0.49
1:B:472:HIS:HD1	1:B:473:PRO:HA	1.77	0.49
1:D:267:LEU:HD13	1:D:267:LEU:N	2.27	0.49
1:D:407:TRP:CB	1:D:418:ASN:HD21	2.22	0.49
1:E:162:GLY:O	1:E:335:ILE:HD11	2.12	0.49
1:C:163:GLU:O	1:C:164:ARG:HG2	2.12	0.49
1:C:209:LEU:HD12	1:C:214:LEU:HD12	1.94	0.49
1:E:413:VAL:N	1:E:414:PRO:CD	2.75	0.49
1:E:460:LEU:HA	1:F:458:CYS:SG	2.53	0.49
1:F:371:PRO:O	1:F:371:PRO:HG2	2.12	0.49
1:F:380:TYR:CD1	1:F:381:GLY:N	2.80	0.49
1:B:319:THR:HG21	1:B:323:GLN:HB3	1.93	0.49
1:C:43:PHE:HD1	1:C:44:VAL:O	1.95	0.49
1:C:225:LEU:HD12	1:C:225:LEU:N	2.27	0.49
1:C:232:MET:O	1:C:233:ALA:C	2.48	0.49
1:D:249:ARG:HB3	1:D:250:GLN:NE2	2.27	0.49
1:E:119:ALA:O	1:E:123:LYS:HG3	2.12	0.49
1:F:270:THR:HG22	1:F:280:ILE:HG22	1.94	0.49
1:F:395:GLY:O	1:F:396:GLU:C	2.51	0.49
1:A:295:SER:HB3	1:A:335:ILE:CD1	2.39	0.49
1:C:205:CYS:C	1:C:207:GLY:N	2.66	0.49
1:C:239:HIS:CE1	1:C:378:LEU:HG	2.48	0.49
1:D:409:LEU:HD12	1:D:409:LEU:O	2.12	0.49
1:E:404:SER:CB	1:E:478:ILE:HD11	2.40	0.49
1:F:180:SER:O	1:F:181:ASP:C	2.51	0.49
1:A:387:GLU:HA	1:A:426:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:LEU:HD12	1:C:225:LEU:H	1.78	0.49
1:C:342:LEU:HB2	1:C:345:VAL:HG21	1.93	0.49
1:D:270:THR:CG2	1:D:280:ILE:HG22	2.43	0.49
1:D:317:PRO:O	1:D:318:VAL:CG1	2.61	0.49
1:E:470:GLY:O	1:F:344:PRO:HG2	2.13	0.49
1:B:141:MET:HE3	1:B:149:GLU:HG2	1.94	0.49
1:C:188:TYR:HD2	1:C:263:THR:HG22	1.75	0.49
1:C:401:VAL:HG22	1:C:486:LYS:HB2	1.93	0.49
1:D:454:ALA:O	1:D:457:LYS:HB2	2.13	0.49
1:E:406:PHE:CE2	1:E:421:CYS:HB3	2.45	0.49
1:E:418:ASN:ND2	1:E:419:ASN:N	2.60	0.49
1:A:55:LEU:HD13	1:A:116:TYR:HB3	1.93	0.49
1:A:78:GLN:HE21	1:A:416:ARG:HH11	1.53	0.49
1:B:163:GLU:OE2	1:B:334:ASP:HB3	2.13	0.49
1:C:30:GLU:HA	1:C:33:LYS:HD3	1.95	0.49
1:D:13:PHE:CE2	1:D:39:MET:HB2	2.47	0.49
1:D:380:TYR:OH	1:D:439:HIS:HD2	1.95	0.49
1:F:472:HIS:ND1	1:F:473:PRO:CA	2.76	0.49
1:A:451:GLY:HA2	1:B:452:PHE:CE1	2.48	0.49
1:C:328:TYR:CD1	1:C:328:TYR:C	2.85	0.49
1:C:494:GLN:O	1:C:495:SER:O	2.30	0.49
1:D:317:PRO:C	1:D:318:VAL:CG1	2.80	0.49
1:E:361:SER:OG	1:E:363:VAL:HG23	2.13	0.49
1:A:68:LYS:NZ	1:B:473:PRO:O	2.41	0.49
1:A:428:ASN:ND2	1:A:431:ASP:HB3	2.28	0.49
1:B:150:LYS:HG2	1:B:152:TYR:CZ	2.48	0.49
1:B:268:LYS:NZ	1:B:280:ILE:HD12	2.28	0.49
1:E:376:THR:O	1:E:377:PRO:C	2.50	0.49
1:E:418:ASN:HD21	1:E:495:SER:HB3	1.77	0.49
1:E:499:GLY:HA3	1:F:29:LYS:HZ3	1.78	0.49
1:F:438:PHE:CE2	1:F:449:THR:HG23	2.48	0.49
1:A:134:PHE:HB2	1:A:301:GLY:O	2.13	0.49
1:A:217:THR:HA	1:A:246:LYS:O	2.12	0.49
1:B:168:LEU:HD11	1:B:291:VAL:HG11	1.94	0.49
1:D:173:ASP:HB2	1:D:289:LEU:HD11	1.94	0.49
1:D:291:VAL:O	1:D:291:VAL:CG1	2.59	0.49
1:D:411:TRP:O	1:D:414:PRO:HD2	2.12	0.49
1:E:163:GLU:OE2	1:E:334:ASP:HB3	2.13	0.49
1:A:472:HIS:O	2:B:600:FAD:N3	2.46	0.48
1:C:153:SER:CB	4:C:2002:HOH:O	2.57	0.48
1:D:67:LYS:CD	1:D:204:GLU:OE1	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:195:VAL:HG22	1:F:288:LEU:HB3	1.94	0.48
1:A:13:PHE:O	1:A:154:ALA:HA	2.12	0.48
1:A:443:PRO:O	1:A:444:ASN:HB2	2.12	0.48
1:B:303:GLU:OE1	1:B:304:THR:HG23	2.13	0.48
1:B:434:ARG:HG2	1:B:434:ARG:HH11	1.79	0.48
1:C:192:LYS:HE2	1:C:215:ASP:CG	2.32	0.48
1:C:305:VAL:HG11	1:C:329:ILE:HD11	1.95	0.48
1:C:328:TYR:C	1:C:328:TYR:HD1	2.17	0.48
1:D:229:ASP:C	1:D:229:ASP:OD1	2.52	0.48
1:A:97:ASP:C	1:A:97:ASP:OD1	2.51	0.48
1:B:65:ILE:HB	1:B:66:PRO:HD2	1.95	0.48
1:B:91:GLU:O	1:B:92:ASP:C	2.51	0.48
1:B:263:THR:CB	1:B:264:PRO:HD3	2.42	0.48
1:C:172:GLY:HA3	1:C:256:ILE:CG2	2.42	0.48
1:C:316:ILE:CG2	1:C:324:THR:CG2	2.91	0.48
1:C:474:VAL:HG12	1:D:447:GLU:OE1	2.13	0.48
1:D:275:ASN:ND2	1:D:277:GLU:HB3	2.28	0.48
1:E:425:VAL:HG13	1:E:435:VAL:HG13	1.95	0.48
1:F:412:THR:O	1:F:415:SER:N	2.46	0.48
1:A:64:CYS:O	1:A:65:ILE:C	2.50	0.48
1:A:212:ILE:HA	1:A:212:ILE:HD12	1.28	0.48
1:B:390:ALA:HB2	1:B:426:ILE:HD12	1.96	0.48
1:B:401:VAL:O	1:B:401:VAL:HG12	2.13	0.48
1:C:43:PHE:HB2	1:C:130:ALA:C	2.33	0.48
1:C:83:SER:HB3	1:C:88:TRP:HB2	1.96	0.48
1:C:114:TRP:CZ3	1:C:117:ARG:HD2	2.48	0.48
1:C:411:TRP:O	1:C:414:PRO:HD2	2.12	0.48
1:C:438:PHE:CE2	1:C:452:PHE:CB	2.96	0.48
1:E:447:GLU:CD	1:F:474:VAL:HG13	2.33	0.48
1:F:478:ILE:HD13	1:F:479:PHE:N	2.28	0.48
1:A:263:THR:HG1	1:A:264:PRO:HD3	1.76	0.48
1:B:374:VAL:CG1	1:B:380:TYR:HB3	2.43	0.48
1:C:72:GLN:OE1	1:C:72:GLN:HA	2.14	0.48
1:D:426:ILE:HG13	1:D:426:ILE:O	2.13	0.48
1:F:208:PHE:CE1	1:F:209:LEU:HD13	2.49	0.48
1:B:70:MET:SD	1:B:101:MET:HE1	2.53	0.48
1:B:259:ILE:HD11	1:B:268:LYS:HB2	1.95	0.48
1:C:166:ARG:HD3	1:C:294:ASP:OD1	2.13	0.48
1:C:233:ALA:O	1:C:236:ILE:HB	2.14	0.48
1:D:78:GLN:HE21	1:D:416:ARG:NH1	2.12	0.48
1:D:209:LEU:O	1:D:212:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LYS:NZ	1:D:276:SER:OG	2.41	0.48
1:E:233:ALA:HA	1:E:236:ILE:HD12	1.96	0.48
1:E:323:GLN:HB2	1:E:330:TYR:CE1	2.49	0.48
1:E:325:ASN:ND2	1:E:325:ASN:H	2.10	0.48
1:F:486:LYS:O	1:F:488:SER:N	2.46	0.48
1:F:491:ASP:OD2	1:F:493:LEU:HB2	2.13	0.48
1:C:255:LYS:HZ2	1:C:270:THR:HG21	1.79	0.48
1:C:477:GLU:O	1:C:478:ILE:C	2.47	0.48
1:D:191:GLY:HA3	1:D:285:ASN:HD22	1.78	0.48
1:D:267:LEU:N	1:D:267:LEU:CD1	2.75	0.48
1:D:272:LYS:HG2	1:D:273:SER:N	2.28	0.48
1:D:407:TRP:CZ3	1:D:412:THR:HG22	2.49	0.48
1:E:267:LEU:O	1:E:283:GLU:HA	2.13	0.48
1:E:418:ASN:HD22	1:E:419:ASN:H	1.62	0.48
1:E:499:GLY:HA3	1:F:29:LYS:NZ	2.29	0.48
1:F:340:LEU:HG	1:F:370:VAL:HG21	1.95	0.48
1:A:267:LEU:N	1:A:267:LEU:CD2	2.74	0.48
1:B:448:VAL:HG22	1:B:476:ALA:HB2	1.94	0.48
1:C:178:ILE:HB	1:C:182:ASP:CB	2.43	0.48
1:C:258:GLN:NE2	1:C:260:GLU:O	2.47	0.48
1:E:173:ASP:OD1	1:E:173:ASP:C	2.52	0.48
1:E:308:LYS:N	1:E:325:ASN:HD21	1.99	0.48
1:F:368:ASP:O	1:F:457:LYS:NZ	2.46	0.48
1:D:402:TYR:HB3	1:D:482:LEU:HB3	1.95	0.48
1:D:402:TYR:N	1:D:402:TYR:CD1	2.82	0.48
1:D:407:TRP:CB	1:D:418:ASN:ND2	2.77	0.48
1:F:221:ARG:HH12	3:F:601:NDP:P2B	2.36	0.48
1:B:284:PHE:N	1:B:284:PHE:CD1	2.82	0.47
1:B:374:VAL:O	1:B:374:VAL:CG1	2.62	0.47
1:E:426:ILE:CG1	1:E:437:GLY:CA	2.88	0.47
1:E:473:PRO:O	1:E:473:PRO:CG	2.56	0.47
1:F:263:THR:OG1	1:F:264:PRO:CD	2.62	0.47
1:F:406:PHE:CE1	1:F:421:CYS:CB	2.94	0.47
1:A:331:ALA:O	1:A:332:ILE:HG12	2.14	0.47
1:C:134:PHE:HB2	1:C:301:GLY:O	2.13	0.47
1:C:205:CYS:O	1:C:207:GLY:N	2.47	0.47
1:C:229:ASP:C	1:C:229:ASP:OD1	2.53	0.47
1:E:273:SER:HB2	1:E:275:ASN:OD1	2.14	0.47
1:A:470:GLY:CA	1:B:450:GLN:HE22	2.25	0.47
1:B:205:CYS:HA	1:B:208:PHE:CE2	2.49	0.47
1:B:273:SER:OG	1:B:275:ASN:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:CYS:HA	1:C:434:ARG:O	2.14	0.47
1:D:378:LEU:HD11	1:D:442:GLY:HA2	1.96	0.47
1:E:178:ILE:HB	1:E:182:ASP:HB2	1.96	0.47
1:E:223:ILE:CD1	1:E:230:GLN:NE2	2.77	0.47
1:F:194:LEU:HD22	1:F:284:PHE:CE1	2.49	0.47
1:F:221:ARG:HH11	1:F:221:ARG:CB	2.27	0.47
1:A:348:GLN:HE22	1:A:351:ARG:HH12	1.57	0.47
1:B:383:CYS:SG	1:B:456:LEU:HD12	2.54	0.47
1:C:395:GLY:O	1:C:396:GLU:C	2.52	0.47
1:D:150:LYS:HG2	1:D:152:TYR:CZ	2.48	0.47
1:D:394:PHE:CE2	1:D:428:ASN:ND2	2.82	0.47
1:F:196:VAL:O	1:F:291:VAL:HG23	2.13	0.47
1:F:223:ILE:HG12	1:F:230:GLN:NE2	2.28	0.47
1:A:353:LEU:HA	1:A:356:ARG:HH21	1.78	0.47
1:C:167:TYR:HD2	1:C:173:ASP:O	1.98	0.47
1:C:321:GLU:O	1:C:322:GLU:HB2	2.13	0.47
1:C:403:HIS:CD2	1:C:492:ILE:HD11	2.48	0.47
1:F:34:PHE:CZ	1:F:355:GLN:NE2	2.83	0.47
1:F:303:GLU:N	1:F:303:GLU:OE1	2.48	0.47
1:B:395:GLY:O	1:B:396:GLU:C	2.52	0.47
1:C:220:VAL:HG23	1:C:250:GLN:H	1.79	0.47
1:D:133:LYS:O	1:D:140:ILE:HG13	2.15	0.47
1:E:16:ILE:HB	1:E:157:PHE:CE1	2.50	0.47
1:E:263:THR:O	1:E:265:GLY:N	2.47	0.47
1:E:305:VAL:HG11	1:E:329:ILE:HD11	1.97	0.47
1:A:47:THR:HG23	1:A:51:THR:O	2.15	0.47
1:A:83:SER:HB2	1:A:88:TRP:HB2	1.97	0.47
1:A:273:SER:OG	1:A:275:ASN:N	2.46	0.47
1:C:67:LYS:NZ	1:C:204:GLU:OE2	2.47	0.47
1:C:127:TYR:CD1	1:C:128:GLU:N	2.82	0.47
1:C:320:ASP:O	1:C:364:LYS:CG	2.49	0.47
1:D:352:LEU:O	1:D:355:GLN:HB2	2.15	0.47
1:E:30:GLU:OE1	1:E:355:GLN:NE2	2.45	0.47
1:E:212:ILE:HA	1:E:212:ILE:HD12	1.55	0.47
1:E:263:THR:CB	1:E:264:PRO:HD3	2.18	0.47
1:F:203:LEU:HD22	1:F:240:MET:CE	2.44	0.47
1:A:11:TYR:CE2	1:A:155:GLU:HG3	2.50	0.47
1:A:395:GLY:O	1:A:396:GLU:C	2.53	0.47
1:B:236:ILE:HG21	1:B:376:THR:HG21	1.96	0.47
1:C:371:PRO:HB3	1:C:453:ALA:HB2	1.97	0.47
1:D:343:THR:CB	1:D:344:PRO:HD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:387:GLU:O	1:F:391:VAL:HG13	2.14	0.47
1:A:163:GLU:OE2	1:A:334:ASP:HB3	2.15	0.47
1:A:191:GLY:O	1:A:193:THR:HG22	2.15	0.47
1:A:471:ILE:HG13	1:B:371:PRO:HB2	1.97	0.47
1:A:475:CYS:O	1:A:478:ILE:HD11	2.15	0.47
1:C:18:ILE:HD11	1:C:159:ILE:CG2	2.45	0.47
1:C:70:MET:HB3	1:C:208:PHE:CE2	2.50	0.47
1:C:398:ASN:O	1:C:429:LEU:HB2	2.15	0.47
1:C:431:ASP:O	1:C:432:ASN:HB2	2.14	0.47
1:C:477:GLU:CA	1:D:450:GLN:HE21	2.24	0.47
1:F:65:ILE:HD13	1:F:65:ILE:HA	1.71	0.47
1:F:273:SER:HB2	1:F:274:THR:H	1.51	0.47
1:F:469:ILE:HD12	1:F:469:ILE:H	1.79	0.47
1:A:348:GLN:HE22	1:A:351:ARG:CZ	2.24	0.47
1:B:9:LYS:HD2	1:B:9:LYS:O	2.14	0.47
1:C:36:LYS:HE3	1:C:358:TYR:CD2	2.48	0.47
1:C:198:ALA:HB1	1:C:224:LEU:HA	1.97	0.47
1:C:221:ARG:NH1	3:C:601:NDP:O2X	2.48	0.47
1:D:220:VAL:CG2	1:D:249:ARG:HE	2.28	0.47
1:D:388:GLU:O	1:D:391:VAL:HG22	2.15	0.47
1:F:223:ILE:HG12	1:F:224:LEU:N	2.29	0.47
1:B:30:GLU:O	1:B:31:ALA:C	2.53	0.46
1:B:98:TRP:HB3	1:B:189:CYS:HB2	1.97	0.46
1:C:316:ILE:CG2	1:C:324:THR:HG21	2.45	0.46
1:C:319:THR:OG1	1:C:323:GLN:O	2.33	0.46
1:C:474:VAL:HG12	1:C:475:CYS:N	2.29	0.46
1:D:47:THR:HB	1:D:48:PRO:HD2	1.96	0.46
1:D:440:VAL:O	1:D:440:VAL:HG13	2.14	0.46
1:E:186:LEU:HD22	1:E:188:TYR:CE2	2.50	0.46
1:E:378:LEU:HD11	1:E:442:GLY:HA2	1.96	0.46
1:F:418:ASN:O	1:F:420:LYS:HG2	2.15	0.46
1:A:292:GLY:O	1:A:293:ARG:HG2	2.15	0.46
1:A:491:ASP:OD2	1:A:493:LEU:HB2	2.15	0.46
1:D:114:TRP:CE3	1:D:114:TRP:O	2.68	0.46
1:F:91:GLU:O	1:F:91:GLU:HG2	2.14	0.46
1:F:413:VAL:N	1:F:414:PRO:CD	2.77	0.46
1:B:220:VAL:HG21	1:B:249:ARG:NE	2.31	0.46
1:B:229:ASP:HB2	1:B:386:SER:HB2	1.98	0.46
1:B:426:ILE:CG1	1:B:437:GLY:CA	2.89	0.46
1:C:21:GLY:HA3	2:C:600:FAD:O3P	2.16	0.46
1:D:376:THR:HB	1:D:377:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:TYR:CE1	1:E:382:CYS:HB3	2.50	0.46
1:A:158:LEU:HD11	1:A:332:ILE:HG12	1.95	0.46
1:A:307:VAL:HG13	1:A:324:THR:HG21	1.97	0.46
1:A:425:VAL:HG13	1:A:435:VAL:HG13	1.96	0.46
1:B:229:ASP:OD1	1:B:231:ASP:N	2.48	0.46
1:B:254:THR:HG23	1:B:271:ALA:HA	1.97	0.46
1:B:482:LEU:HA	1:B:482:LEU:HD23	1.40	0.46
1:C:32:ALA:HB2	1:C:125:VAL:CG2	2.46	0.46
1:C:386:SER:OG	1:C:388:GLU:HG2	2.15	0.46
1:D:230:GLN:HB2	1:D:388:GLU:OE2	2.15	0.46
1:D:316:ILE:HG13	1:D:335:ILE:CG2	2.45	0.46
1:D:407:TRP:CD1	1:D:418:ASN:ND2	2.82	0.46
1:E:203:LEU:HD23	1:E:203:LEU:HA	1.56	0.46
1:F:229:ASP:OD2	1:F:232:MET:HG2	2.15	0.46
1:A:30:GLU:OE1	1:A:33:LYS:HD2	2.15	0.46
1:A:47:THR:HG1	1:A:51:THR:H	1.63	0.46
1:A:263:THR:O	1:A:264:PRO:C	2.50	0.46
1:B:47:THR:HB	1:B:48:PRO:CD	2.46	0.46
1:C:307:VAL:HG21	1:C:329:ILE:HG21	1.97	0.46
1:C:412:THR:HB	1:D:108:HIS:CD2	2.50	0.46
1:D:98:TRP:NE1	1:D:102:THR:CG2	2.72	0.46
1:A:134:PHE:CE1	1:A:157:PHE:CD2	3.04	0.46
1:A:348:GLN:NE2	1:A:351:ARG:CZ	2.79	0.46
1:B:356:ARG:HG2	1:B:361:SER:O	2.15	0.46
1:C:55:LEU:HD13	1:C:116:TYR:CB	2.44	0.46
1:D:96:HIS:NE2	1:D:212:ILE:HG13	2.30	0.46
1:D:270:THR:HG21	1:D:280:ILE:HG22	1.97	0.46
1:E:134:PHE:HE1	1:E:157:PHE:CD2	2.34	0.46
1:A:469:ILE:HD13	1:A:469:ILE:N	2.31	0.46
1:B:23:GLY:HA3	1:B:332:ILE:HD13	1.98	0.46
1:B:172:GLY:HA2	1:B:175:GLU:HG2	1.96	0.46
1:B:374:VAL:HG12	1:B:380:TYR:HB3	1.97	0.46
1:C:158:LEU:HD11	1:C:332:ILE:HB	1.97	0.46
1:C:309:ILE:CG2	1:C:316:ILE:HG12	2.43	0.46
1:C:433:GLU:O	1:C:434:ARG:C	2.54	0.46
1:A:262:GLY:C	1:A:263:THR:O	2.54	0.46
1:B:164:ARG:NH2	1:B:181:ASP:OD2	2.45	0.46
1:C:194:LEU:HD22	1:C:287:VAL:HG13	1.98	0.46
1:D:90:LEU:N	1:D:90:LEU:CD2	2.78	0.46
1:D:469:ILE:CG2	1:D:470:GLY:N	2.79	0.46
1:E:38:VAL:HG22	1:E:125:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:470:GLY:CA	1:F:480:THR:HG21	2.46	0.46
1:A:284:PHE:CD1	1:A:284:PHE:N	2.84	0.46
1:C:55:LEU:HD11	1:C:116:TYR:HB3	1.97	0.46
1:C:201:VAL:HG22	2:C:600:FAD:HM73	1.97	0.46
1:C:220:VAL:CG2	1:C:249:ARG:NE	2.70	0.46
1:C:293:ARG:NH1	2:C:600:FAD:HM81	2.31	0.46
1:C:393:LYS:HG2	1:C:394:PHE:CE1	2.51	0.46
1:D:258:GLN:HE22	1:D:261:ALA:HB2	1.79	0.46
1:D:263:THR:O	1:D:265:GLY:N	2.49	0.46
1:D:407:TRP:HB2	1:D:418:ASN:ND2	2.24	0.46
1:E:138:HIS:CD2	1:E:154:ALA:O	2.65	0.46
1:A:14:ASP:OD2	1:A:37:LYS:N	2.47	0.46
1:A:471:ILE:HG21	1:B:373:THR:CG2	2.42	0.46
1:A:471:ILE:H	1:B:450:GLN:HE22	1.64	0.46
1:B:49:LEU:HA	1:B:49:LEU:HD13	1.65	0.46
1:B:120:LEU:HD22	1:B:125:VAL:CG1	2.45	0.46
1:C:63:GLY:O	1:C:64:CYS:C	2.53	0.46
1:E:49:LEU:N	1:E:49:LEU:CD2	2.78	0.46
1:E:281:GLU:OE1	1:E:281:GLU:HA	2.14	0.46
1:F:162:GLY:O	1:F:335:ILE:HD11	2.16	0.46
1:A:269:VAL:HG12	1:A:281:GLU:OE1	2.17	0.45
1:B:348:GLN:NE2	1:B:351:ARG:HH12	2.13	0.45
1:B:418:ASN:OD1	1:B:419:ASN:N	2.47	0.45
1:B:461:THR:H	1:B:464:GLN:HG3	1.80	0.45
1:D:90:LEU:CD2	1:D:90:LEU:H	2.29	0.45
1:D:91:GLU:OE1	1:D:91:GLU:HA	2.12	0.45
1:D:140:ILE:CG1	1:D:141:MET:N	2.79	0.45
1:D:225:LEU:O	1:D:226:ARG:C	2.55	0.45
1:D:282:ASP:OD1	1:D:282:ASP:N	2.48	0.45
1:F:498:CYS:SG	1:F:499:GLY:N	2.89	0.45
1:C:225:LEU:O	1:C:228:PHE:HB2	2.16	0.45
1:C:438:PHE:C	1:C:439:HIS:ND1	2.69	0.45
1:C:477:GLU:CA	1:D:450:GLN:NE2	2.73	0.45
1:D:287:VAL:O	1:D:287:VAL:HG12	2.16	0.45
1:F:109:ILE:HA	1:F:112:LEU:HD12	1.99	0.45
1:F:168:LEU:O	1:F:173:ASP:OD2	2.33	0.45
1:F:396:GLU:O	1:F:396:GLU:OE2	2.33	0.45
1:F:428:ASN:ND2	1:F:431:ASP:CB	2.73	0.45
1:C:90:LEU:HG	1:C:91:GLU:N	2.32	0.45
1:C:181:ASP:N	1:C:181:ASP:OD1	2.48	0.45
1:C:255:LYS:HZ3	1:C:270:THR:HG23	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:473:PRO:O	1:C:473:PRO:CG	2.60	0.45
1:D:301:GLY:C	1:D:303:GLU:OE1	2.54	0.45
2:D:600:FAD:O2A	2:D:600:FAD:O5'	2.35	0.45
1:E:164:ARG:HD2	1:E:164:ARG:HA	1.73	0.45
1:A:450:GLN:NE2	1:B:471:ILE:H	2.14	0.45
1:B:305:VAL:HG12	1:B:328:TYR:OH	2.16	0.45
1:E:36:LYS:HA	1:E:36:LYS:HD3	1.76	0.45
1:F:250:GLN:O	1:F:251:PHE:CD1	2.69	0.45
1:F:406:PHE:HE2	1:F:423:ALA:HB2	1.82	0.45
1:F:478:ILE:HD13	1:F:479:PHE:H	1.81	0.45
1:A:114:TRP:HB3	1:D:114:TRP:CE2	2.50	0.45
1:A:220:VAL:O	1:A:220:VAL:CG2	2.65	0.45
1:A:435:VAL:HG23	1:A:460:LEU:O	2.17	0.45
1:E:86:TYR:O	1:F:96:HIS:CE1	2.60	0.45
1:E:219:MET:HE2	1:E:219:MET:HB2	1.69	0.45
1:F:55:LEU:HD22	1:F:56:GLY:N	2.31	0.45
1:B:21:GLY:HA3	2:B:600:FAD:O5B	2.17	0.45
1:B:262:GLY:C	1:B:263:THR:O	2.55	0.45
1:C:98:TRP:HD1	1:C:189:CYS:CA	2.19	0.45
1:C:134:PHE:HB3	1:C:305:VAL:CG2	2.46	0.45
1:C:229:ASP:HB2	1:C:386:SER:HB2	1.99	0.45
1:D:69:LEU:O	1:D:72:GLN:HB3	2.16	0.45
1:D:138:HIS:HD2	1:D:154:ALA:O	1.99	0.45
1:F:292:GLY:O	1:F:293:ARG:HG2	2.16	0.45
1:A:167:TYR:HB3	1:A:173:ASP:OD2	2.17	0.45
1:A:412:THR:O	1:A:415:SER:N	2.48	0.45
1:B:426:ILE:O	1:B:426:ILE:HG13	2.16	0.45
1:C:76:LEU:O	1:C:79:ALA:HB3	2.17	0.45
1:C:291:VAL:CG1	3:C:601:NDP:C8A	2.95	0.45
1:C:342:LEU:O	1:C:345:VAL:HB	2.15	0.45
2:E:600:FAD:H9	2:E:600:FAD:H1'1	1.42	0.45
1:F:318:VAL:HG23	1:F:323:GLN:C	2.37	0.45
1:A:55:LEU:HD23	1:A:55:LEU:HA	1.54	0.45
1:A:357:LEU:HB3	1:A:358:TYR:CD1	2.51	0.45
1:B:17:ILE:HG12	1:B:158:LEU:HD23	1.98	0.45
1:B:65:ILE:CG2	1:B:66:PRO:CD	2.91	0.45
1:B:469:ILE:CG2	1:B:470:GLY:N	2.80	0.45
1:C:100:LYS:O	1:C:100:LYS:HD3	2.16	0.45
1:C:365:CYS:SG	1:C:367:TYR:CE2	3.10	0.45
1:A:134:PHE:HE1	1:A:157:PHE:CD2	2.34	0.45
1:A:403:HIS:CE1	1:A:486:LYS:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HD12	1:B:335:ILE:HA	1.73	0.45
1:C:30:GLU:O	1:C:33:LYS:HB2	2.17	0.45
1:C:167:TYR:CD2	1:C:173:ASP:O	2.70	0.45
1:D:72:GLN:HA	1:D:72:GLN:HE21	1.81	0.45
1:D:84:ARG:HE	1:D:84:ARG:HB2	1.52	0.45
1:D:114:TRP:CE3	1:D:118:VAL:HG23	2.51	0.45
1:D:138:HIS:O	1:D:153:SER:HA	2.17	0.45
1:E:108:HIS:CE1	1:E:112:LEU:HD11	2.52	0.45
1:E:273:SER:OG	1:E:275:ASN:OD1	2.23	0.45
1:E:480:THR:HG22	1:E:481:THR:HG23	1.98	0.45
1:A:176:TYR:HB3	1:A:267:LEU:CD1	2.47	0.45
1:A:195:VAL:HG22	1:A:288:LEU:HB3	1.98	0.45
1:B:216:VAL:CG1	1:B:217:THR:N	2.80	0.45
1:B:230:GLN:NE2	1:B:230:GLN:HA	2.32	0.45
1:C:109:ILE:O	1:C:112:LEU:N	2.50	0.45
1:C:172:GLY:HA3	1:C:256:ILE:HG22	1.99	0.45
1:C:409:LEU:O	1:C:409:LEU:HD12	2.17	0.45
1:E:228:PHE:N	1:E:228:PHE:CD1	2.85	0.45
1:E:408:PRO:HG2	1:E:411:TRP:CD2	2.51	0.45
1:F:150:LYS:HD3	1:F:152:TYR:CZ	2.51	0.45
1:C:415:SER:O	1:C:415:SER:OG	2.29	0.44
1:C:451:GLY:O	1:C:454:ALA:HB3	2.17	0.44
1:E:317:PRO:C	1:E:318:VAL:CG2	2.86	0.44
1:E:318:VAL:HG12	1:E:323:GLN:O	2.16	0.44
1:F:194:LEU:HB2	1:F:284:PHE:CZ	2.52	0.44
1:F:318:VAL:HG21	1:F:322:GLU:HA	1.99	0.44
1:F:472:HIS:CE1	1:F:473:PRO:HB3	2.51	0.44
1:A:471:ILE:CG1	1:B:371:PRO:HB2	2.47	0.44
1:A:496:GLY:C	1:A:497:CYS:SG	2.95	0.44
1:B:55:LEU:CD1	1:B:116:TYR:HB3	2.46	0.44
1:B:98:TRP:CB	1:B:189:CYS:HB2	2.48	0.44
1:B:151:VAL:HG12	1:B:152:TYR:N	2.31	0.44
1:C:58:THR:HG1	2:C:600:FAD:PA	2.40	0.44
1:C:130:ALA:HB1	1:C:143:THR:O	2.17	0.44
1:C:186:LEU:HA	1:C:187:PRO:HD2	1.78	0.44
1:D:309:ILE:HG21	1:D:309:ILE:HD13	1.64	0.44
1:E:266:ARG:NH1	1:E:283:GLU:OE1	2.48	0.44
1:A:117:ARG:NH2	1:D:107:ASN:ND2	2.65	0.44
1:A:413:VAL:N	1:A:414:PRO:CD	2.81	0.44
1:A:487:ARG:HE	1:A:487:ARG:HB2	1.60	0.44
1:B:399:ILE:HD12	1:B:399:ILE:HA	1.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD13	1:C:49:LEU:HA	1.84	0.44
1:C:162:GLY:HA3	2:C:600:FAD:O1A	2.18	0.44
1:F:221:ARG:NH1	1:F:221:ARG:HG2	2.32	0.44
1:F:343:THR:N	1:F:344:PRO:CD	2.80	0.44
1:A:192:LYS:N	1:A:285:ASN:HD22	2.13	0.44
1:A:303:GLU:OE1	1:A:304:THR:HG23	2.17	0.44
1:B:376:THR:O	1:B:377:PRO:C	2.56	0.44
1:C:20:GLY:HA3	1:C:42:ASP:CB	2.47	0.44
1:C:208:PHE:CD1	1:C:208:PHE:C	2.90	0.44
1:D:86:TYR:CZ	1:D:413:VAL:HB	2.51	0.44
1:E:410:GLU:HG3	1:F:72:GLN:NE2	2.31	0.44
1:A:29:LYS:CG	1:A:30:GLU:N	2.79	0.44
1:A:188:TYR:C	1:A:188:TYR:CD1	2.90	0.44
1:A:216:VAL:CG1	1:A:217:THR:N	2.80	0.44
1:A:351:ARG:NH2	1:A:352:LEU:HD21	2.33	0.44
1:B:180:SER:O	1:B:181:ASP:C	2.53	0.44
1:E:269:VAL:O	1:E:281:GLU:HB2	2.17	0.44
1:E:272:LYS:HG2	1:E:273:SER:H	1.82	0.44
1:F:49:LEU:N	1:F:49:LEU:CD2	2.78	0.44
1:A:449:THR:O	1:A:450:GLN:C	2.56	0.44
1:C:98:TRP:CE3	1:C:102:THR:OG1	2.57	0.44
1:C:209:LEU:HD13	1:C:209:LEU:HA	1.67	0.44
1:C:401:VAL:O	1:C:401:VAL:HG23	2.18	0.44
1:C:472:HIS:CD2	1:C:477:GLU:OE2	2.59	0.44
1:D:343:THR:HG22	1:D:344:PRO:HD3	2.00	0.44
1:E:316:ILE:HA	1:E:317:PRO:HD3	1.88	0.44
1:E:412:THR:O	1:E:415:SER:N	2.48	0.44
1:F:42:ASP:HA	2:F:600:FAD:N3A	2.33	0.44
1:F:418:ASN:OD1	1:F:419:ASN:N	2.50	0.44
1:A:275:ASN:CG	1:A:275:ASN:O	2.56	0.44
1:A:408:PRO:O	1:A:409:LEU:C	2.54	0.44
1:A:428:ASN:ND2	1:A:431:ASP:HB2	2.32	0.44
1:C:332:ILE:CG2	1:C:333:GLY:N	2.80	0.44
1:C:427:CYS:HB3	1:C:433:GLU:C	2.38	0.44
1:D:30:GLU:O	1:D:31:ALA:C	2.54	0.44
1:D:76:LEU:HD23	1:D:76:LEU:HA	1.77	0.44
1:E:469:ILE:CG2	1:E:470:GLY:N	2.79	0.44
1:A:161:THR:HB	2:A:600:FAD:C8A	2.48	0.44
1:B:292:GLY:C	1:B:293:ARG:HG2	2.38	0.44
1:C:256:ILE:HG12	1:C:257:GLU:N	2.32	0.44
1:C:425:VAL:CG1	1:C:435:VAL:HG13	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:GLU:O	1:C:480:THR:HG23	2.17	0.44
1:D:186:LEU:HA	1:D:187:PRO:HD3	1.67	0.44
1:D:281:GLU:HA	1:D:281:GLU:OE1	2.17	0.44
1:E:462:LYS:NZ	1:E:482:LEU:O	2.41	0.44
1:F:82:ASP:OD2	1:F:416:ARG:NH1	2.51	0.44
1:A:335:ILE:HD12	1:A:335:ILE:HA	1.79	0.44
1:A:482:LEU:HD23	1:A:482:LEU:HA	1.78	0.44
1:C:65:ILE:HG22	1:C:66:PRO:CD	2.48	0.44
1:C:188:TYR:CD1	1:C:263:THR:O	2.71	0.44
1:C:194:LEU:HD23	1:C:195:VAL:N	2.33	0.44
1:C:239:HIS:CE1	1:C:378:LEU:HB2	2.53	0.44
1:C:461:THR:HG1	1:C:464:GLN:HG3	1.77	0.44
1:D:395:GLY:O	1:D:396:GLU:C	2.56	0.44
1:E:91:GLU:C	1:E:93:THR:H	2.22	0.44
1:E:196:VAL:O	1:E:291:VAL:HG13	2.17	0.44
1:E:200:TYR:O	1:E:201:VAL:C	2.56	0.44
1:E:233:ALA:O	1:E:236:ILE:HB	2.18	0.44
1:A:331:ALA:C	1:A:332:ILE:HG12	2.39	0.43
1:A:422:TYR:HE2	1:A:424:LYS:HE2	1.82	0.43
1:B:68:LYS:O	1:B:71:HIS:HB3	2.18	0.43
1:B:83:SER:HB2	1:B:88:TRP:CD1	2.53	0.43
1:C:196:VAL:O	1:C:291:VAL:HG22	2.14	0.43
1:C:208:PHE:HD1	1:C:209:LEU:N	2.13	0.43
1:C:376:THR:CB	1:C:377:PRO:CD	2.94	0.43
1:D:389:LYS:HD2	1:D:389:LYS:HA	1.83	0.43
1:F:378:LEU:HD11	1:F:442:GLY:HA2	2.00	0.43
1:B:220:VAL:HG21	1:B:249:ARG:HE	1.83	0.43
1:B:305:VAL:HG11	1:B:329:ILE:HD11	2.00	0.43
1:C:30:GLU:O	1:C:31:ALA:C	2.56	0.43
1:C:137:PRO:O	1:C:138:HIS:CB	2.66	0.43
1:C:428:ASN:C	1:C:428:ASN:OD1	2.56	0.43
1:D:403:HIS:CD2	1:D:403:HIS:C	2.91	0.43
1:E:106:GLN:OE1	1:E:185:SER:HB3	2.18	0.43
1:E:373:THR:CG2	1:F:471:ILE:CG2	2.92	0.43
1:E:469:ILE:HG23	1:E:470:GLY:N	2.32	0.43
1:A:91:GLU:O	1:A:92:ASP:C	2.57	0.43
1:A:493:LEU:O	1:A:494:GLN:CG	2.57	0.43
1:B:186:LEU:HD12	1:B:190:PRO:HG3	2.00	0.43
1:E:209:LEU:O	1:E:212:ILE:HG22	2.18	0.43
1:E:438:PHE:C	1:E:439:HIS:ND1	2.71	0.43
1:B:16:ILE:HB	1:B:157:PHE:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:HB3	1:B:339:LYS:HG2	2.00	0.43
1:C:158:LEU:HA	1:C:330:TYR:O	2.18	0.43
1:C:307:VAL:HG13	1:C:325:ASN:HD21	1.84	0.43
1:D:263:THR:CB	1:D:264:PRO:CD	2.96	0.43
1:D:316:ILE:O	1:D:318:VAL:HG13	2.18	0.43
1:D:488:SER:OG	1:D:489:GLY:N	2.51	0.43
1:A:189:CYS:HA	1:A:190:PRO:HD3	1.85	0.43
1:A:307:VAL:HA	1:A:325:ASN:HD21	1.83	0.43
1:B:248:ILE:CD1	1:B:281:GLU:OE2	2.67	0.43
1:B:256:ILE:HD11	1:B:267:LEU:HB3	2.00	0.43
1:B:387:GLU:O	1:B:391:VAL:HG13	2.19	0.43
1:B:387:GLU:HG3	1:B:401:VAL:HG21	2.01	0.43
1:B:443:PRO:O	1:B:444:ASN:C	2.55	0.43
1:C:25:LEU:HD11	1:C:55:LEU:HD22	2.00	0.43
1:C:41:LEU:CD1	1:C:130:ALA:HB3	2.48	0.43
1:C:212:ILE:HD12	1:C:212:ILE:HA	1.78	0.43
1:D:80:LEU:HD23	1:D:80:LEU:HA	1.74	0.43
1:D:331:ALA:O	1:D:332:ILE:HD13	2.19	0.43
1:E:88:TRP:HE3	1:F:94:VAL:HG12	1.83	0.43
1:E:475:CYS:HB2	1:F:447:GLU:OE1	2.19	0.43
1:F:90:LEU:HD23	1:F:90:LEU:HA	1.55	0.43
1:F:235:LYS:HE2	1:F:422:TYR:CD2	2.53	0.43
1:B:411:TRP:CD1	1:B:411:TRP:N	2.85	0.43
1:C:98:TRP:NE1	1:C:190:PRO:CD	2.49	0.43
1:D:212:ILE:HD12	1:D:212:ILE:HA	1.57	0.43
1:A:13:PHE:HE2	1:A:152:TYR:CD2	2.37	0.43
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.55	0.43
1:A:122:GLU:OE1	1:A:122:GLU:HA	2.18	0.43
1:B:45:THR:HA	1:B:46:PRO:HD3	1.73	0.43
1:B:318:VAL:HG22	1:B:323:GLN:C	2.39	0.43
1:B:319:THR:C	1:B:321:GLU:H	2.21	0.43
1:B:454:ALA:O	1:B:457:LYS:HB2	2.18	0.43
3:B:601:NDP:H8A	3:B:601:NDP:H51A	2.00	0.43
1:D:396:GLU:C	1:D:396:GLU:CD	2.77	0.43
1:F:225:LEU:HD12	1:F:228:PHE:CD2	2.53	0.43
1:A:18:ILE:HG21	1:A:18:ILE:HD13	1.72	0.43
1:B:465:LEU:HD21	1:B:479:PHE:O	2.19	0.43
1:B:478:ILE:H	1:B:478:ILE:HG13	1.35	0.43
1:C:161:THR:N	1:C:335:ILE:HD11	2.33	0.43
1:C:166:ARG:HB2	1:C:294:ASP:OD1	2.19	0.43
1:C:413:VAL:N	1:C:414:PRO:CD	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:413:VAL:N	1:D:414:PRO:HD3	2.34	0.43
1:E:375:PHE:CD1	1:E:375:PHE:N	2.87	0.43
1:F:141:MET:HE3	1:F:143:THR:OG1	2.19	0.43
1:F:209:LEU:HA	1:F:209:LEU:HD12	1.63	0.43
1:F:325:ASN:ND2	1:F:325:ASN:N	2.51	0.43
1:A:280:ILE:HG13	1:A:280:ILE:O	2.19	0.43
1:A:292:GLY:C	1:A:293:ARG:HG2	2.39	0.43
1:B:209:LEU:HB3	1:B:216:VAL:HG21	1.99	0.43
1:C:313:THR:OG1	1:C:314:GLY:N	2.52	0.43
1:D:195:VAL:HG22	1:D:288:LEU:HB2	2.00	0.43
1:E:90:LEU:HA	1:E:90:LEU:HD23	1.74	0.43
1:E:140:ILE:O	1:E:140:ILE:CG2	2.67	0.43
1:E:228:PHE:O	1:E:230:GLN:N	2.50	0.43
1:F:185:SER:O	1:F:186:LEU:C	2.55	0.43
1:F:318:VAL:CG2	1:F:323:GLN:O	2.67	0.43
1:F:422:TYR:CE1	1:F:424:LYS:HB3	2.48	0.43
1:A:144:ASN:OD1	1:A:146:LYS:N	2.51	0.43
1:C:343:THR:N	1:C:344:PRO:CD	2.82	0.43
1:D:185:SER:O	1:D:186:LEU:C	2.57	0.43
1:D:232:MET:CE	1:D:441:LEU:HB2	2.49	0.43
1:E:192:LYS:HG3	1:E:215:ASP:OD1	2.19	0.43
1:E:373:THR:HG21	1:E:446:GLY:CA	2.47	0.43
1:F:217:THR:HA	1:F:246:LYS:O	2.19	0.43
1:A:273:SER:OG	1:A:274:THR:N	2.49	0.42
1:A:475:CYS:O	1:A:478:ILE:CD1	2.66	0.42
1:A:487:ARG:O	1:A:487:ARG:HG3	2.17	0.42
1:C:237:GLY:O	1:C:238:GLU:C	2.54	0.42
1:D:80:LEU:O	1:D:83:SER:OG	2.36	0.42
2:D:600:FAD:H1'1	2:D:600:FAD:H9	1.81	0.42
1:E:257:GLU:H	1:E:257:GLU:HG2	1.72	0.42
1:E:335:ILE:HD12	1:E:335:ILE:HA	1.76	0.42
1:F:47:THR:HB	1:F:48:PRO:HD2	2.00	0.42
1:F:438:PHE:CE1	1:F:479:PHE:CZ	3.07	0.42
2:F:600:FAD:O2A	2:F:600:FAD:O5'	2.37	0.42
1:A:282:ASP:O	1:A:284:PHE:CE1	2.72	0.42
1:A:325:ASN:O	1:A:327:PRO:HD3	2.19	0.42
1:B:74:ALA:HA	1:B:212:ILE:CD1	2.50	0.42
1:B:403:HIS:CD2	1:B:492:ILE:CD1	3.01	0.42
1:E:17:ILE:HG12	1:E:158:LEU:HD23	2.00	0.42
1:E:168:LEU:N	1:E:168:LEU:CD1	2.81	0.42
1:E:310:ASN:ND2	1:E:313:THR:HG23	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:323:GLN:CA	1:F:330:TYR:CD1	2.98	0.42
1:A:371:PRO:HB2	1:B:471:ILE:HD11	2.01	0.42
1:B:60:VAL:HG13	1:B:112:LEU:CD1	2.49	0.42
2:B:600:FAD:H9	2:B:600:FAD:H1'1	1.65	0.42
1:C:18:ILE:HG21	1:C:18:ILE:HD13	1.73	0.42
1:C:189:CYS:C	1:C:191:GLY:N	2.72	0.42
1:D:411:TRP:CZ2	1:D:443:PRO:HG3	2.54	0.42
1:E:488:SER:O	1:E:489:GLY:C	2.55	0.42
1:F:223:ILE:HD11	1:F:230:GLN:CG	2.49	0.42
1:C:34:PHE:HZ	1:C:355:GLN:HE22	1.68	0.42
1:C:70:MET:HG3	1:C:101:MET:HE1	2.01	0.42
1:C:278:GLU:C	1:C:278:GLU:CD	2.78	0.42
1:D:114:TRP:CE3	1:D:118:VAL:CG2	3.01	0.42
1:D:158:LEU:HA	1:D:330:TYR:O	2.20	0.42
1:E:21:GLY:HA2	1:E:57:GLY:HA3	2.02	0.42
1:E:203:LEU:HD22	1:E:240:MET:HE1	2.00	0.42
1:E:380:TYR:OH	1:E:439:HIS:HD2	2.02	0.42
1:F:217:THR:HG23	1:F:246:LYS:CB	2.48	0.42
1:A:106:GLN:O	1:A:107:ASN:C	2.56	0.42
1:A:334:ASP:OD2	2:A:600:FAD:H5'1	2.20	0.42
1:B:168:LEU:N	1:B:168:LEU:CD1	2.81	0.42
1:B:292:GLY:O	1:B:293:ARG:HG2	2.19	0.42
1:C:134:PHE:CG	1:C:305:VAL:HG21	2.54	0.42
1:C:183:LEU:C	1:C:185:SER:N	2.70	0.42
1:C:212:ILE:O	1:C:212:ILE:HG23	2.18	0.42
1:C:224:LEU:H	1:C:224:LEU:CD1	2.01	0.42
1:D:114:TRP:HE3	1:D:118:VAL:HG23	1.84	0.42
1:D:223:ILE:HG12	1:D:226:ARG:NH2	2.34	0.42
1:F:163:GLU:HB3	1:F:294:ASP:C	2.40	0.42
1:F:221:ARG:CG	1:F:221:ARG:NH1	2.80	0.42
1:A:163:GLU:HB3	1:A:294:ASP:C	2.40	0.42
1:B:106:GLN:O	1:B:107:ASN:C	2.57	0.42
1:B:403:HIS:O	1:B:403:HIS:HD2	2.03	0.42
1:C:40:VAL:HG12	1:C:126:VAL:O	2.18	0.42
1:C:274:THR:O	1:C:274:THR:OG1	2.34	0.42
1:C:291:VAL:HG13	3:C:601:NDP:C8A	2.49	0.42
1:C:336:LEU:HD23	1:C:336:LEU:HA	1.79	0.42
1:C:348:GLN:NE2	1:C:352:LEU:HD22	2.34	0.42
1:D:43:PHE:HD2	1:D:130:ALA:HA	1.85	0.42
1:D:186:LEU:HA	1:D:186:LEU:HD23	1.71	0.42
1:D:194:LEU:HD22	1:D:284:PHE:CZ	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:303:GLU:N	1:D:303:GLU:CD	2.56	0.42
1:D:334:ASP:OD1	2:D:600:FAD:H5'2	2.20	0.42
1:F:351:ARG:NH2	1:F:352:LEU:HD21	2.35	0.42
1:A:112:LEU:O	1:A:113:ASN:C	2.57	0.42
1:A:316:ILE:HA	1:A:317:PRO:HD3	1.88	0.42
1:B:22:SER:HG	1:B:343:THR:HG23	1.83	0.42
1:B:161:THR:HB	2:B:600:FAD:C8A	2.49	0.42
1:B:272:LYS:HG2	1:B:273:SER:N	2.35	0.42
1:C:365:CYS:SG	1:C:365:CYS:O	2.77	0.42
1:C:429:LEU:HD12	1:C:429:LEU:HA	1.70	0.42
1:C:473:PRO:HG2	1:D:68:LYS:HD3	2.01	0.42
1:D:41:LEU:N	1:D:41:LEU:HD23	2.35	0.42
1:D:400:GLU:HG2	1:D:429:LEU:CD1	2.44	0.42
1:E:96:HIS:CD2	1:E:212:ILE:HG13	2.55	0.42
1:E:173:ASP:CG	1:E:174:LYS:N	2.71	0.42
1:F:186:LEU:HD22	1:F:186:LEU:HA	1.71	0.42
1:F:208:PHE:O	1:F:209:LEU:C	2.57	0.42
1:F:426:ILE:CD1	1:F:436:VAL:CG2	2.92	0.42
1:A:45:THR:HA	1:A:46:PRO:HD3	1.81	0.42
1:B:144:ASN:CG	1:B:145:ASN:N	2.72	0.42
1:C:192:LYS:O	1:C:192:LYS:HG2	2.18	0.42
1:C:373:THR:OG1	1:D:471:ILE:HG21	2.19	0.42
1:D:86:TYR:HE1	1:D:414:PRO:HG3	1.84	0.42
1:D:494:GLN:HE21	1:D:494:GLN:HB2	1.72	0.42
1:F:60:VAL:CG1	1:F:112:LEU:HD13	2.49	0.42
1:F:131:TYR:CD1	1:F:131:TYR:C	2.92	0.42
1:A:58:THR:O	1:A:63:GLY:N	2.53	0.42
1:A:67:LYS:NZ	1:A:204:GLU:CD	2.73	0.42
1:A:85:ASN:HB2	1:A:413:VAL:HG12	2.02	0.42
1:A:267:LEU:O	1:A:283:GLU:CB	2.68	0.42
1:A:323:GLN:NE2	1:A:327:PRO:HA	2.35	0.42
1:B:16:ILE:HD13	1:B:16:ILE:HG21	1.77	0.42
1:B:168:LEU:CD1	1:B:291:VAL:HG11	2.49	0.42
1:B:432:ASN:O	1:B:433:GLU:HB2	2.20	0.42
1:C:164:ARG:HH11	1:C:165:PRO:HD2	1.85	0.42
1:C:422:TYR:CE1	1:C:424:LYS:HB3	2.55	0.42
1:D:200:TYR:O	1:D:201:VAL:C	2.58	0.42
1:D:221:ARG:HB2	1:D:252:VAL:HG22	2.01	0.42
1:D:233:ALA:O	1:D:236:ILE:HB	2.20	0.42
1:D:407:TRP:CE3	1:D:412:THR:HG22	2.54	0.42
1:E:67:LYS:HB3	1:E:67:LYS:HE2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:112:LEU:O	1:E:113:ASN:C	2.59	0.42
1:F:12:ASP:HB2	1:F:153:SER:O	2.20	0.42
1:F:195:VAL:HG22	1:F:288:LEU:CB	2.50	0.42
1:F:321:GLU:HG2	1:F:356:ARG:NH1	2.35	0.42
1:A:263:THR:CB	1:A:264:PRO:CD	2.97	0.42
1:A:429:LEU:HD23	1:A:433:GLU:HG2	2.02	0.42
1:B:47:THR:HG21	1:B:182:ASP:OD1	2.20	0.42
1:C:34:PHE:HZ	1:C:355:GLN:NE2	2.18	0.42
1:C:85:ASN:OD1	1:C:85:ASN:N	2.52	0.42
1:C:98:TRP:HE1	1:C:190:PRO:CD	2.23	0.42
1:D:343:THR:HB	1:D:344:PRO:HD2	1.99	0.42
1:D:478:ILE:HD12	1:D:479:PHE:H	1.84	0.42
3:D:601:NDP:O2N	3:D:601:NDP:O2A	2.38	0.42
1:E:55:LEU:HD13	1:E:116:TYR:HB3	2.02	0.42
1:E:302:LEU:HA	1:E:302:LEU:HD23	1.75	0.42
1:E:313:THR:C	1:E:315:LYS:H	2.20	0.42
1:E:371:PRO:HB2	1:F:471:ILE:CD1	2.44	0.42
1:E:426:ILE:CD1	1:E:436:VAL:HG23	2.49	0.42
1:F:72:GLN:HG3	1:F:76:LEU:HD22	2.01	0.42
1:F:189:CYS:HA	1:F:190:PRO:HD3	1.96	0.42
1:C:191:GLY:O	1:C:193:THR:N	2.53	0.41
1:C:325:ASN:ND2	1:C:325:ASN:N	2.68	0.41
1:D:343:THR:CG2	1:D:344:PRO:HD3	2.50	0.41
1:F:178:ILE:HB	1:F:182:ASP:HB2	2.02	0.41
1:F:221:ARG:NH1	3:F:601:NDP:P2B	2.93	0.41
1:A:383:CYS:SG	1:A:456:LEU:HD12	2.60	0.41
1:B:221:ARG:NH1	3:B:601:NDP:C4A	2.83	0.41
1:C:21:GLY:HA2	1:C:57:GLY:CA	2.50	0.41
1:C:53:TRP:HB2	1:C:61:ASN:OD1	2.20	0.41
1:C:67:LYS:NZ	1:C:204:GLU:CD	2.73	0.41
1:C:401:VAL:CG2	1:C:486:LYS:HB2	2.50	0.41
1:D:195:VAL:HG22	1:D:288:LEU:CB	2.50	0.41
1:E:431:ASP:OD1	1:E:431:ASP:C	2.58	0.41
1:E:471:ILE:HD12	1:F:450:GLN:HB2	2.02	0.41
1:E:474:VAL:O	1:E:475:CYS:C	2.58	0.41
1:E:497:CYS:SG	1:F:112:LEU:CD2	3.08	0.41
1:F:158:LEU:HD22	1:F:353:LEU:HD23	2.02	0.41
1:F:168:LEU:HD21	1:F:253:PRO:HG2	2.02	0.41
1:A:176:TYR:HB3	1:A:267:LEU:HD12	2.02	0.41
1:A:191:GLY:O	1:A:193:THR:HG23	2.19	0.41
1:A:225:LEU:HD23	1:A:225:LEU:HA	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:THR:HG23	1:B:62:VAL:HG23	2.02	0.41
1:B:491:ASP:OD1	1:B:493:LEU:HG	2.19	0.41
1:C:43:PHE:CD1	1:C:44:VAL:O	2.73	0.41
1:C:88:TRP:CZ3	1:D:96:HIS:HB2	2.55	0.41
1:C:326:VAL:HA	1:C:327:PRO:HD2	1.92	0.41
2:C:600:FAD:H1'1	2:C:600:FAD:H9	1.79	0.41
1:E:370:VAL:O	1:E:370:VAL:CG2	2.67	0.41
1:F:221:ARG:HH11	1:F:221:ARG:HB3	1.85	0.41
1:F:291:VAL:O	3:F:601:NDP:H52A	2.19	0.41
1:F:318:VAL:HG22	1:F:319:THR:H	1.85	0.41
1:F:318:VAL:HG22	1:F:319:THR:N	2.34	0.41
1:F:493:LEU:O	1:F:494:GLN:CG	2.64	0.41
1:A:91:GLU:HG3	1:A:93:THR:H	1.85	0.41
1:A:403:HIS:ND1	1:A:422:TYR:OH	2.39	0.41
1:A:471:ILE:H	1:B:450:GLN:NE2	2.19	0.41
1:B:464:GLN:O	1:B:467:SER:OG	2.25	0.41
1:C:69:LEU:HD23	1:C:69:LEU:HA	1.85	0.41
1:C:179:SER:N	1:C:182:ASP:HB2	2.27	0.41
1:C:272:LYS:HG3	1:C:273:SER:H	1.85	0.41
1:C:277:GLU:OE1	1:C:277:GLU:HA	2.20	0.41
1:D:176:TYR:CE1	1:D:258:GLN:OE1	2.74	0.41
1:E:269:VAL:HG12	1:E:270:THR:N	2.35	0.41
1:E:332:ILE:HD11	1:E:349:ALA:HB1	2.01	0.41
1:E:388:GLU:HG2	1:E:389:LYS:N	2.34	0.41
1:E:395:GLY:O	1:E:396:GLU:C	2.59	0.41
1:E:440:VAL:O	1:E:440:VAL:HG13	2.19	0.41
1:F:72:GLN:HG3	1:F:72:GLN:O	2.20	0.41
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.26	0.41
1:A:318:VAL:HG13	1:A:322:GLU:CA	2.49	0.41
1:B:175:GLU:CD	1:B:175:GLU:H	2.24	0.41
1:B:308:LYS:N	1:B:325:ASN:HD21	2.14	0.41
1:C:183:LEU:HD21	1:C:209:LEU:HD21	2.02	0.41
1:C:267:LEU:N	1:C:267:LEU:HD23	2.35	0.41
1:C:297:THR:HG21	1:C:316:ILE:HD11	2.01	0.41
1:E:440:VAL:HG22	1:E:441:LEU:N	2.35	0.41
1:F:288:LEU:HD22	1:F:290:ALA:H	1.86	0.41
1:F:438:PHE:HE2	1:F:449:THR:HG23	1.84	0.41
1:B:86:TYR:CE2	1:B:414:PRO:HD3	2.54	0.41
1:B:185:SER:O	1:B:186:LEU:C	2.58	0.41
1:C:452:PHE:O	1:C:455:ALA:N	2.53	0.41
1:C:478:ILE:HD12	1:C:478:ILE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:401:VAL:HG22	1:D:426:ILE:HB	2.03	0.41
1:E:305:VAL:HG11	1:E:329:ILE:CD1	2.49	0.41
1:F:137:PRO:O	1:F:139:LYS:N	2.53	0.41
1:F:313:THR:C	1:F:315:LYS:H	2.15	0.41
1:A:450:GLN:HE22	1:B:470:GLY:CA	2.32	0.41
1:B:336:LEU:HB3	1:B:339:LYS:CG	2.51	0.41
1:B:402:TYR:CD1	1:B:402:TYR:N	2.89	0.41
1:C:27:ALA:O	1:C:28:ALA:C	2.59	0.41
1:C:72:GLN:O	1:C:73:ALA:C	2.57	0.41
1:C:422:TYR:CD1	1:C:422:TYR:C	2.94	0.41
1:D:21:GLY:HA3	2:D:600:FAD:O5B	2.20	0.41
1:E:158:LEU:HA	1:E:330:TYR:O	2.21	0.41
1:F:109:ILE:HG22	1:F:113:ASN:HD21	1.86	0.41
1:F:212:ILE:HD12	1:F:212:ILE:HA	1.67	0.41
1:F:319:THR:C	1:F:321:GLU:H	2.23	0.41
1:F:406:PHE:CZ	1:F:421:CYS:HB3	2.56	0.41
1:C:168:LEU:HD12	1:C:168:LEU:HA	1.66	0.41
1:C:188:TYR:O	1:C:190:PRO:CD	2.66	0.41
1:D:232:MET:HE1	1:D:441:LEU:HB2	2.03	0.41
1:D:460:LEU:HD21	1:D:465:LEU:HD13	2.03	0.41
1:E:45:THR:HA	1:E:46:PRO:HD3	1.78	0.41
1:E:497:CYS:SG	1:F:112:LEU:HD22	2.61	0.41
1:F:91:GLU:O	1:F:92:ASP:C	2.58	0.41
2:F:600:FAD:H8A	2:F:600:FAD:H2B	1.79	0.41
1:A:21:GLY:HA2	1:A:57:GLY:HA3	2.02	0.41
1:A:34:PHE:CE2	1:A:359:GLY:CA	3.03	0.41
1:A:136:GLY:O	1:A:137:PRO:C	2.59	0.41
1:A:170:ILE:HB	1:A:254:THR:O	2.21	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.78	0.41
1:A:274:THR:H	1:A:274:THR:HG23	1.48	0.41
1:A:371:PRO:HB3	1:A:453:ALA:HB2	2.03	0.41
1:A:386:SER:HB3	1:A:389:LYS:HB2	2.03	0.41
1:B:194:LEU:HB2	1:B:284:PHE:CE2	2.56	0.41
1:B:403:HIS:CD2	1:B:403:HIS:C	2.94	0.41
1:C:42:ASP:HA	2:C:600:FAD:N3A	2.36	0.41
1:C:65:ILE:C	1:C:67:LYS:N	2.73	0.41
1:C:170:ILE:O	1:C:173:ASP:OD1	2.39	0.41
1:C:260:GLU:CB	1:C:266:ARG:HB3	2.51	0.41
1:C:322:GLU:O	1:C:330:TYR:HD2	2.03	0.41
1:C:440:VAL:O	1:C:440:VAL:HG13	2.20	0.41
1:D:91:GLU:O	1:D:92:ASP:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:278:GLU:OE2	1:D:280:ILE:HG23	2.21	0.41
1:D:367:TYR:CD1	1:D:367:TYR:N	2.88	0.41
1:D:397:GLU:H	1:D:397:GLU:HG2	1.54	0.41
1:E:255:LYS:HE3	1:E:270:THR:HG21	2.03	0.41
1:E:361:SER:OG	1:E:362:THR:N	2.54	0.41
1:F:475:CYS:O	1:F:477:GLU:N	2.54	0.41
1:F:489:GLY:O	1:F:490:GLY:O	2.37	0.41
1:A:343:THR:O	1:A:347:ILE:HG23	2.21	0.41
1:A:344:PRO:HG3	1:B:472:HIS:HB2	2.02	0.41
1:A:382:CYS:HA	1:A:438:PHE:O	2.21	0.41
1:B:64:CYS:O	1:B:65:ILE:C	2.59	0.41
1:C:58:THR:HG21	1:C:293:ARG:HH22	1.86	0.41
1:D:288:LEU:HA	1:D:288:LEU:HD23	1.78	0.41
1:D:386:SER:OG	1:D:389:LYS:HB2	2.21	0.41
1:D:472:HIS:HA	1:D:473:PRO:HA	1.82	0.41
1:E:163:GLU:HB3	1:E:295:SER:HA	2.03	0.41
1:F:101:MET:O	1:F:105:VAL:HG23	2.21	0.41
1:F:475:CYS:O	1:F:476:ALA:C	2.59	0.41
1:C:20:GLY:CA	1:C:42:ASP:HB2	2.51	0.40
1:C:337:GLU:O	1:C:339:LYS:HG2	2.21	0.40
1:D:163:GLU:HB3	1:D:295:SER:CA	2.46	0.40
1:D:366:ASP:C	1:D:366:ASP:OD1	2.59	0.40
1:D:411:TRP:NE1	1:D:416:ARG:NH2	2.69	0.40
1:E:342:LEU:O	1:E:345:VAL:HB	2.20	0.40
1:F:39:MET:SD	1:F:41:LEU:HD21	2.61	0.40
1:F:65:ILE:HB	1:F:66:PRO:HD3	2.02	0.40
1:B:221:ARG:HD3	3:B:601:NDP:C2A	2.51	0.40
1:C:70:MET:HB3	1:C:208:PHE:CD2	2.57	0.40
1:C:170:ILE:HD12	1:C:254:THR:C	2.42	0.40
1:C:474:VAL:CG1	1:D:447:GLU:CD	2.89	0.40
1:D:67:LYS:HE2	1:D:67:LYS:HB3	1.84	0.40
1:D:430:LYS:HE3	1:D:430:LYS:HB2	1.52	0.40
1:E:386:SER:O	1:E:387:GLU:C	2.56	0.40
1:A:402:TYR:CD1	1:A:462:LYS:HE2	2.56	0.40
1:B:228:PHE:O	1:B:229:ASP:C	2.60	0.40
1:D:292:GLY:HA2	3:D:601:NDP:O2N	2.21	0.40
1:D:382:CYS:HA	1:D:438:PHE:O	2.20	0.40
1:E:86:TYR:O	1:F:101:MET:HB2	2.22	0.40
1:E:136:GLY:O	1:E:137:PRO:C	2.59	0.40
1:F:166:ARG:HG3	1:F:294:ASP:OD2	2.21	0.40
1:F:221:ARG:HH11	1:F:221:ARG:HG2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:302:LEU:HD23	1:F:302:LEU:HA	1.76	0.40
1:F:413:VAL:HB	1:F:414:PRO:HD3	2.04	0.40
1:A:42:ASP:OD1	2:A:600:FAD:H1B	2.22	0.40
1:A:185:SER:O	1:A:186:LEU:C	2.59	0.40
1:A:195:VAL:HB	1:A:218:VAL:HG22	2.03	0.40
1:A:497:CYS:SG	1:B:112:LEU:HD22	2.61	0.40
1:B:267:LEU:O	1:B:283:GLU:HA	2.21	0.40
1:B:371:PRO:HD3	1:B:383:CYS:SG	2.61	0.40
1:C:461:THR:HG23	1:C:464:GLN:OE1	2.21	0.40
1:D:21:GLY:HA2	1:D:57:GLY:HA3	2.03	0.40
1:D:61:ASN:C	1:D:62:VAL:CG1	2.89	0.40
1:D:324:THR:HB	1:D:325:ASN:HD22	1.84	0.40
1:D:332:ILE:HA	1:D:332:ILE:HD12	1.53	0.40
1:E:309:ILE:HD13	1:E:309:ILE:HG21	1.58	0.40
1:F:123:LYS:O	1:F:124:LYS:HB2	2.21	0.40
1:A:154:ALA:HB3	1:A:157:PHE:CE1	2.56	0.40
1:A:309:ILE:HA	1:A:317:PRO:HD3	2.04	0.40
1:A:318:VAL:CG1	1:A:322:GLU:CA	2.89	0.40
1:C:31:ALA:C	1:C:33:LYS:N	2.69	0.40
1:D:9:LYS:HB3	1:D:11:TYR:CE1	2.57	0.40
1:D:193:THR:HG22	1:D:194:LEU:N	2.37	0.40
1:D:209:LEU:HA	1:D:209:LEU:HD12	1.75	0.40
1:D:332:ILE:HD11	1:D:349:ALA:HB1	2.03	0.40
1:E:232:MET:HE2	1:E:232:MET:HB3	1.95	0.40
1:E:258:GLN:HA	1:E:267:LEU:HD12	2.04	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	488/499 (98%)	445 (91%)	36 (7%)	7 (1%)	11 43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	485/499 (97%)	436 (90%)	40 (8%)	9 (2%)	8	36
1	C	480/499 (96%)	395 (82%)	70 (15%)	15 (3%)	4	23
1	D	485/499 (97%)	439 (90%)	37 (8%)	9 (2%)	8	36
1	E	489/499 (98%)	441 (90%)	39 (8%)	9 (2%)	8	37
1	F	488/499 (98%)	438 (90%)	40 (8%)	10 (2%)	7	34
All	All	2915/2994 (97%)	2594 (89%)	262 (9%)	59 (2%)	7	34

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	THR
1	A	489	GLY
1	B	92	ASP
1	B	263	THR
1	B	314	GLY
1	B	489	GLY
1	C	32	ALA
1	C	184	PHE
1	C	190	PRO
1	C	191	GLY
1	C	192	LYS
1	C	489	GLY
1	D	92	ASP
1	D	263	THR
1	D	314	GLY
1	D	489	GLY
1	E	263	THR
1	E	314	GLY
1	E	489	GLY
1	F	263	THR
1	F	314	GLY
1	A	314	GLY
1	C	287	VAL
1	E	92	ASP
1	E	283	GLU
1	F	92	ASP
1	F	283	GLU
1	F	487	ARG
1	F	490	GLY
1	A	92	ASP

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Mol	Chain	Res	Type
1	C	206	ALA
1	C	327	PRO
1	C	396	GLU
1	D	144	ASN
1	D	494	GLN
1	E	229	ASP
1	F	144	ASN
1	F	229	ASP
1	A	229	ASP
1	A	291	VAL
1	C	44	VAL
1	C	113	ASN
1	D	35	ASP
1	D	229	ASP
1	E	35	ASP
1	A	35	ASP
1	B	144	ASN
1	B	282	ASP
1	B	229	ASP
1	B	291	VAL
1	C	62	VAL
1	E	291	VAL
1	F	488	SER
1	F	291	VAL
1	D	291	VAL
1	E	62	VAL
1	C	264	PRO
1	B	62	VAL
1	C	473	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	406/414 (98%)	352 (87%)	54 (13%)	4 17
1	B	405/414 (98%)	344 (85%)	61 (15%)	3 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	400/414 (97%)	325 (81%)	75 (19%)	1 8
1	D	405/414 (98%)	342 (84%)	63 (16%)	2 13
1	E	407/414 (98%)	354 (87%)	53 (13%)	4 19
1	F	406/414 (98%)	349 (86%)	57 (14%)	3 16
All	All	2429/2484 (98%)	2066 (85%)	363 (15%)	3 14

All (363) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASP
1	A	38	VAL
1	A	40	VAL
1	A	55	LEU
1	A	64	CYS
1	A	76	LEU
1	A	85	ASN
1	A	94	VAL
1	A	99	GLU
1	A	102	THR
1	A	107	ASN
1	A	144	ASN
1	A	163	GLU
1	A	166	ARG
1	A	168	LEU
1	A	179	SER
1	A	185	SER
1	A	193	THR
1	A	209	LEU
1	A	212	ILE
1	A	221	ARG
1	A	245	ILE
1	A	246	LYS
1	A	257	GLU
1	A	259	ILE
1	A	267	LEU
1	A	270	THR
1	A	282	ASP
1	A	283	GLU
1	A	303	GLU
1	A	305	VAL
1	A	309	ILE

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Mol	Chain	Res	Type
1	A	310	ASN
1	A	324	THR
1	A	335	ILE
1	A	347	ILE
1	A	356	ARG
1	A	358	TYR
1	A	361	SER
1	A	363	VAL
1	A	364	LYS
1	A	365	CYS
1	A	372	THR
1	A	373	THR
1	A	399	ILE
1	A	403	HIS
1	A	416	ARG
1	A	426	ILE
1	A	434	ARG
1	A	461	THR
1	A	469	ILE
1	A	473	PRO
1	A	478	ILE
1	A	487	ARG
1	B	9	LYS
1	B	22	SER
1	B	39	MET
1	B	40	VAL
1	B	51	THR
1	B	55	LEU
1	B	64	CYS
1	B	67	LYS
1	B	76	LEU
1	B	84	ARG
1	B	89	LYS
1	B	91	GLU
1	B	92	ASP
1	B	99	GLU
1	B	107	ASN
1	B	111	SER
1	B	129	ASN
1	B	150	LYS
1	B	163	GLU
1	B	168	LEU

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Mol	Chain	Res	Type
1	B	185	SER
1	B	186	LEU
1	B	209	LEU
1	B	212	ILE
1	B	220	VAL
1	B	221	ARG
1	B	223	ILE
1	B	256	ILE
1	B	257	GLU
1	B	263	THR
1	B	268	LYS
1	B	272	LYS
1	B	276	SER
1	B	278	GLU
1	B	280	ILE
1	B	282	ASP
1	B	288	LEU
1	B	293	ARG
1	B	297	THR
1	B	303	GLU
1	B	305	VAL
1	B	310	ASN
1	B	318	VAL
1	B	325	ASN
1	B	335	ILE
1	B	336	LEU
1	B	340	LEU
1	B	344	PRO
1	B	347	ILE
1	B	348	GLN
1	B	373	THR
1	B	391	VAL
1	B	397	GLU
1	B	399	ILE
1	B	403	HIS
1	B	416	ARG
1	B	464	GLN
1	B	469	ILE
1	B	478	ILE
1	B	487	ARG
1	B	494	GLN
1	C	33	LYS

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Mol	Chain	Res	Type
1	C	37	LYS
1	C	45	THR
1	C	52	ASN
1	C	55	LEU
1	C	64	CYS
1	C	98	TRP
1	C	100	LYS
1	C	102	THR
1	C	104	SER
1	C	129	ASN
1	C	135	ILE
1	C	138	HIS
1	C	139	LYS
1	C	141	MET
1	C	143	THR
1	C	152	TYR
1	C	153	SER
1	C	159	ILE
1	C	161	THR
1	C	163	GLU
1	C	168	LEU
1	C	175	GLU
1	C	178	ILE
1	C	180	SER
1	C	181	ASP
1	C	193	THR
1	C	209	LEU
1	C	212	ILE
1	C	220	VAL
1	C	224	LEU
1	C	234	ASN
1	C	255	LYS
1	C	258	GLN
1	C	259	ILE
1	C	260	GLU
1	C	263	THR
1	C	267	LEU
1	C	269	VAL
1	C	273	SER
1	C	274	THR
1	C	276	SER
1	C	278	GLU

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Mol	Chain	Res	Type
1	C	283	GLU
1	C	285	ASN
1	C	288	LEU
1	C	289	LEU
1	C	294	ASP
1	C	297	THR
1	C	310	ASN
1	C	312	LYS
1	C	318	VAL
1	C	319	THR
1	C	324	THR
1	C	325	ASN
1	C	327	PRO
1	C	328	TYR
1	C	347	ILE
1	C	352	LEU
1	C	363	VAL
1	C	365	CYS
1	C	372	THR
1	C	376	THR
1	C	378	LEU
1	C	385	LEU
1	C	389	LYS
1	C	397	GLU
1	C	399	ILE
1	C	403	HIS
1	C	404	SER
1	C	429	LEU
1	C	441	LEU
1	C	469	ILE
1	C	478	ILE
1	C	488	SER
1	D	52	ASN
1	D	55	LEU
1	D	64	CYS
1	D	78	GLN
1	D	84	ARG
1	D	85	ASN
1	D	89	LYS
1	D	90	LEU
1	D	91	GLU
1	D	92	ASP

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Mol	Chain	Res	Type
1	D	102	THR
1	D	123	LYS
1	D	139	LYS
1	D	168	LEU
1	D	185	SER
1	D	186	LEU
1	D	209	LEU
1	D	212	ILE
1	D	220	VAL
1	D	221	ARG
1	D	250	GLN
1	D	251	PHE
1	D	256	ILE
1	D	263	THR
1	D	266	ARG
1	D	267	LEU
1	D	268	LYS
1	D	272	LYS
1	D	276	SER
1	D	277	GLU
1	D	278	GLU
1	D	282	ASP
1	D	283	GLU
1	D	284	PHE
1	D	288	LEU
1	D	291	VAL
1	D	303	GLU
1	D	305	VAL
1	D	325	ASN
1	D	332	ILE
1	D	347	ILE
1	D	364	LYS
1	D	365	CYS
1	D	370	VAL
1	D	372	THR
1	D	373	THR
1	D	376	THR
1	D	382	CYS
1	D	396	GLU
1	D	403	HIS
1	D	409	LEU
1	D	410	GLU

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Mol	Chain	Res	Type
1	D	416	ARG
1	D	418	ASN
1	D	426	ILE
1	D	430	LYS
1	D	436	VAL
1	D	473	PRO
1	D	478	ILE
1	D	485	THR
1	D	492	ILE
1	D	493	LEU
1	D	494	GLN
1	E	22	SER
1	E	29	LYS
1	E	38	VAL
1	E	40	VAL
1	E	52	ASN
1	E	55	LEU
1	E	64	CYS
1	E	72	GLN
1	E	76	LEU
1	E	104	SER
1	E	107	ASN
1	E	133	LYS
1	E	163	GLU
1	E	168	LEU
1	E	173	ASP
1	E	185	SER
1	E	193	THR
1	E	200	TYR
1	E	209	LEU
1	E	212	ILE
1	E	215	ASP
1	E	219	MET
1	E	221	ARG
1	E	228	PHE
1	E	266	ARG
1	E	267	LEU
1	E	275	ASN
1	E	276	SER
1	E	277	GLU
1	E	288	LEU
1	E	291	VAL

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Mol	Chain	Res	Type
1	E	297	THR
1	E	303	GLU
1	E	308	LYS
1	E	309	ILE
1	E	318	VAL
1	E	335	ILE
1	E	336	LEU
1	E	347	ILE
1	E	362	THR
1	E	370	VAL
1	E	373	THR
1	E	391	VAL
1	E	403	HIS
1	E	415	SER
1	E	416	ARG
1	E	434	ARG
1	E	450	GLN
1	E	473	PRO
1	E	478	ILE
1	E	480	THR
1	E	491	ASP
1	E	498	CYS
1	F	29	LYS
1	F	40	VAL
1	F	55	LEU
1	F	58	THR
1	F	64	CYS
1	F	67	LYS
1	F	76	LEU
1	F	81	LYS
1	F	89	LYS
1	F	91	GLU
1	F	92	ASP
1	F	99	GLU
1	F	102	THR
1	F	104	SER
1	F	107	ASN
1	F	139	LYS
1	F	163	GLU
1	F	168	LEU
1	F	170	ILE
1	F	175	GLU

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Mol	Chain	Res	Type
1	F	185	SER
1	F	186	LEU
1	F	193	THR
1	F	209	LEU
1	F	212	ILE
1	F	220	VAL
1	F	221	ARG
1	F	223	ILE
1	F	225	LEU
1	F	250	GLN
1	F	254	THR
1	F	256	ILE
1	F	257	GLU
1	F	267	LEU
1	F	275	ASN
1	F	276	SER
1	F	277	GLU
1	F	282	ASP
1	F	288	LEU
1	F	303	GLU
1	F	308	LYS
1	F	325	ASN
1	F	332	ILE
1	F	347	ILE
1	F	364	LYS
1	F	365	CYS
1	F	391	VAL
1	F	396	GLU
1	F	403	HIS
1	F	404	SER
1	F	416	ARG
1	F	422	TYR
1	F	426	ILE
1	F	434	ARG
1	F	463	GLN
1	F	478	ILE
1	F	497	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN

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Mol	Chain	Res	Type
1	A	78	GLN
1	A	96	HIS
1	A	113	ASN
1	A	138	HIS
1	A	250	GLN
1	A	285	ASN
1	A	310	ASN
1	A	325	ASN
1	A	348	GLN
1	A	418	ASN
1	A	439	HIS
1	A	450	GLN
1	B	96	HIS
1	B	106	GLN
1	B	107	ASN
1	B	113	ASN
1	B	129	ASN
1	B	138	HIS
1	B	239	HIS
1	B	285	ASN
1	B	310	ASN
1	B	325	ASN
1	B	439	HIS
1	B	450	GLN
1	C	72	GLN
1	C	96	HIS
1	C	129	ASN
1	C	138	HIS
1	C	230	GLN
1	C	234	ASN
1	C	250	GLN
1	C	258	GLN
1	C	285	ASN
1	C	310	ASN
1	C	325	ASN
1	C	348	GLN
1	C	355	GLN
1	C	418	ASN
1	C	439	HIS
1	C	444	ASN
1	C	472	HIS
1	D	52	ASN

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	72	GLN
1	D	78	GLN
1	D	106	GLN
1	D	107	ASN
1	D	108	HIS
1	D	138	HIS
1	D	144	ASN
1	D	250	GLN
1	D	275	ASN
1	D	285	ASN
1	D	325	ASN
1	D	403	HIS
1	D	418	ASN
1	D	439	HIS
1	D	472	HIS
1	D	494	GLN
1	E	72	GLN
1	E	113	ASN
1	E	138	HIS
1	E	285	ASN
1	E	323	GLN
1	E	325	ASN
1	E	418	ASN
1	E	419	ASN
1	E	439	HIS
1	E	450	GLN
1	F	71	HIS
1	F	72	GLN
1	F	78	GLN
1	F	96	HIS
1	F	107	ASN
1	F	113	ASN
1	F	138	HIS
1	F	230	GLN
1	F	234	ASN
1	F	250	GLN
1	F	258	GLN
1	F	285	ASN
1	F	325	ASN
1	F	355	GLN
1	F	428	ASN

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Mol	Chain	Res	Type
1	F	439	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	D	600	-	53,58,58	1.56	8 (15%)	68,89,89	1.84	16 (23%)
2	FAD	E	600	-	53,58,58	1.43	6 (11%)	68,89,89	1.92	20 (29%)
3	NDP	B	601	-	36,42,52	1.77	9 (25%)	43,65,80	1.52	9 (20%)
3	NDP	C	601	-	36,42,52	1.56	8 (22%)	43,65,80	1.72	10 (23%)
2	FAD	C	600	-	53,58,58	1.31	5 (9%)	68,89,89	1.87	18 (26%)
2	FAD	B	600	-	53,58,58	1.35	7 (13%)	68,89,89	1.94	17 (25%)
3	NDP	A	601	-	36,42,52	1.49	5 (13%)	43,65,80	1.57	7 (16%)
3	NDP	E	601	-	36,42,52	1.48	6 (16%)	43,65,80	1.33	4 (9%)
3	NDP	D	601	-	36,42,52	1.45	5 (13%)	43,65,80	1.67	9 (20%)
2	FAD	F	600	-	53,58,58	1.22	5 (9%)	68,89,89	1.56	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NDP	F	601	-	36,42,52	1.55	7 (19%)	43,65,80	1.43	8 (18%)
2	FAD	A	600	-	53,58,58	1.31	5 (9%)	68,89,89	1.78	15 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	D	600	-	-	5/30/50/50	0/6/6/6
2	FAD	E	600	-	-	10/30/50/50	0/6/6/6
3	NDP	B	601	-	-	9/23/56/77	0/4/4/5
3	NDP	C	601	-	-	5/23/56/77	0/4/4/5
2	FAD	C	600	-	-	10/30/50/50	0/6/6/6
2	FAD	B	600	-	-	3/30/50/50	0/6/6/6
3	NDP	A	601	-	-	13/23/56/77	0/4/4/5
3	NDP	E	601	-	-	5/23/56/77	0/4/4/5
3	NDP	D	601	-	-	12/23/56/77	0/4/4/5
2	FAD	F	600	-	-	10/30/50/50	0/6/6/6
3	NDP	F	601	-	-	6/23/56/77	0/4/4/5
2	FAD	A	600	-	-	9/30/50/50	0/6/6/6

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	C2A-N3A	4.49	1.39	1.32
2	E	600	FAD	C2A-N3A	4.48	1.39	1.32
2	B	600	FAD	C2A-N3A	4.41	1.39	1.32
2	D	600	FAD	C2A-N3A	4.29	1.39	1.32
3	C	601	NDP	P2B-O3X	4.17	1.70	1.54
2	C	600	FAD	C4X-N5	4.12	1.38	1.30
3	B	601	NDP	P2B-O3X	4.11	1.70	1.54
3	B	601	NDP	C2A-N1A	4.05	1.41	1.33
3	A	601	NDP	P2B-O2X	4.03	1.70	1.54
2	C	600	FAD	C2A-N3A	4.00	1.38	1.32
2	E	600	FAD	C4X-N5	3.90	1.38	1.30
3	B	601	NDP	P2B-O2X	3.87	1.69	1.54
2	F	600	FAD	C4X-N5	3.84	1.38	1.30
3	E	601	NDP	P2B-O2X	3.84	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	601	NDP	P2B-O3X	3.76	1.69	1.54
3	F	601	NDP	P2B-O3X	3.76	1.69	1.54
3	F	601	NDP	P2B-O2X	3.70	1.69	1.54
3	D	601	NDP	P2B-O3X	3.68	1.69	1.54
2	F	600	FAD	C2A-N3A	3.67	1.38	1.32
3	C	601	NDP	P2B-O2X	3.62	1.68	1.54
2	A	600	FAD	C4X-N5	3.62	1.37	1.30
2	D	600	FAD	C2B-C1B	-3.59	1.48	1.53
3	D	601	NDP	P2B-O2X	3.58	1.68	1.54
3	A	601	NDP	PN-O2N	3.57	1.72	1.55
2	D	600	FAD	C2A-N1A	3.55	1.40	1.33
3	B	601	NDP	C5A-C4A	3.51	1.50	1.40
3	E	601	NDP	PA-O2A	3.48	1.71	1.55
3	A	601	NDP	P2B-O3X	3.38	1.67	1.54
3	A	601	NDP	PA-O2A	3.27	1.70	1.55
2	B	600	FAD	C4X-N5	3.26	1.37	1.30
2	D	600	FAD	C5'-C4'	3.23	1.56	1.51
3	D	601	NDP	PN-O2N	3.23	1.70	1.55
3	D	601	NDP	C5A-C4A	3.19	1.49	1.40
3	D	601	NDP	PA-O2A	3.18	1.70	1.55
3	E	601	NDP	PN-O2N	3.18	1.70	1.55
3	C	601	NDP	PN-O2N	3.17	1.70	1.55
3	F	601	NDP	PN-O2N	3.16	1.70	1.55
3	C	601	NDP	PA-O2A	3.16	1.70	1.55
3	F	601	NDP	PA-O2A	3.14	1.70	1.55
3	B	601	NDP	PA-O2A	3.09	1.69	1.55
2	B	600	FAD	C2A-N1A	3.06	1.39	1.33
3	A	601	NDP	C5A-C4A	2.99	1.48	1.40
3	B	601	NDP	C2A-N3A	2.97	1.36	1.32
2	D	600	FAD	C4X-N5	2.88	1.36	1.30
2	F	600	FAD	C2A-N1A	2.83	1.39	1.33
3	B	601	NDP	PN-O2N	2.82	1.68	1.55
3	F	601	NDP	C5A-C4A	2.82	1.48	1.40
2	D	600	FAD	C9A-N10	-2.79	1.36	1.41
2	B	600	FAD	C4X-C10	-2.79	1.35	1.44
2	A	600	FAD	C2A-N1A	2.68	1.38	1.33
2	E	600	FAD	C2B-C1B	-2.60	1.49	1.53
2	C	600	FAD	C5'-C4'	2.57	1.55	1.51
3	E	601	NDP	C5A-C4A	2.57	1.47	1.40
3	C	601	NDP	C5A-C4A	2.53	1.47	1.40
2	C	600	FAD	C2A-N1A	2.49	1.38	1.33
3	F	601	NDP	O4B-C1B	2.44	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	601	NDP	C2A-N3A	2.44	1.36	1.32
3	B	601	NDP	C6A-C5A	2.43	1.52	1.43
2	D	600	FAD	C4X-C10	-2.41	1.37	1.44
2	C	600	FAD	C10-N1	2.40	1.38	1.33
3	C	601	NDP	P2B-O2B	2.35	1.63	1.59
2	F	600	FAD	C10-N1	2.34	1.38	1.33
2	A	600	FAD	C4X-C10	-2.29	1.37	1.44
2	D	600	FAD	O4B-C1B	2.27	1.44	1.41
2	E	600	FAD	C2A-N1A	2.26	1.38	1.33
2	E	600	FAD	C9A-N10	-2.26	1.37	1.41
3	B	601	NDP	C6A-N6A	2.19	1.42	1.34
3	E	601	NDP	C4A-N3A	-2.18	1.32	1.35
3	C	601	NDP	O4B-C1B	2.12	1.44	1.41
2	F	600	FAD	C2B-C1B	-2.11	1.50	1.53
2	A	600	FAD	C9A-C5X	-2.10	1.37	1.41
2	B	600	FAD	C5'-C4'	2.09	1.54	1.51
2	E	600	FAD	C10-N1	2.08	1.37	1.33
2	B	600	FAD	O4B-C4B	-2.08	1.40	1.45
3	F	601	NDP	C6A-C5A	2.07	1.51	1.43
2	B	600	FAD	C2B-C1B	-2.01	1.50	1.53

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	FAD	P-O3P-PA	-6.71	109.79	132.83
2	D	600	FAD	P-O3P-PA	-6.11	111.86	132.83
2	B	600	FAD	N3A-C2A-N1A	-5.76	119.68	128.68
2	C	600	FAD	N3A-C2A-N1A	-5.64	119.87	128.68
2	F	600	FAD	N3A-C2A-N1A	-5.56	119.99	128.68
2	E	600	FAD	C5X-C9A-N10	5.47	123.61	117.95
2	D	600	FAD	N3A-C2A-N1A	-5.35	120.32	128.68
2	C	600	FAD	P-O3P-PA	-5.23	114.88	132.83
3	A	601	NDP	PN-O3-PA	-5.13	115.23	132.83
2	B	600	FAD	C4-N3-C2	-5.07	116.27	125.64
2	A	600	FAD	N3A-C2A-N1A	-5.03	120.81	128.68
2	B	600	FAD	P-O3P-PA	-4.90	116.01	132.83
3	D	601	NDP	PN-O3-PA	-4.69	116.73	132.83
3	C	601	NDP	O3B-C3B-C4B	-4.69	97.50	111.05
2	B	600	FAD	O3B-C3B-C4B	-4.59	97.78	111.05
2	D	600	FAD	C4X-C10-N10	4.53	123.10	116.48
2	E	600	FAD	N3A-C2A-N1A	-4.44	121.74	128.68
2	F	600	FAD	P-O3P-PA	-4.36	117.86	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	FAD	C2B-C3B-C4B	-4.32	94.25	102.64
2	B	600	FAD	O4-C4-C4X	-4.19	115.50	126.60
3	D	601	NDP	N3A-C2A-N1A	-4.02	122.39	128.68
3	E	601	NDP	C1B-N9A-C4A	-3.98	119.64	126.64
2	E	600	FAD	C9A-C5X-N5	-3.87	118.22	122.43
3	B	601	NDP	PN-O3-PA	-3.81	119.77	132.83
2	E	600	FAD	C4-N3-C2	-3.80	118.61	125.64
3	F	601	NDP	N3A-C2A-N1A	-3.79	122.75	128.68
2	D	600	FAD	C4-N3-C2	-3.78	118.66	125.64
2	D	600	FAD	O4B-C1B-C2B	-3.77	101.41	106.93
2	E	600	FAD	P-O3P-PA	-3.75	119.95	132.83
2	E	600	FAD	C9-C9A-N10	-3.68	116.86	121.84
3	C	601	NDP	C3B-C2B-C1B	-3.68	95.97	102.89
3	D	601	NDP	C2A-N1A-C6A	3.67	125.02	118.75
3	E	601	NDP	N3A-C2A-N1A	-3.61	123.04	128.68
2	B	600	FAD	C4X-C4-N3	3.60	122.33	113.19
2	B	600	FAD	C4X-C10-N1	-3.46	116.71	124.73
2	F	600	FAD	O4B-C1B-C2B	-3.45	101.88	106.93
2	C	600	FAD	O4B-C1B-C2B	-3.40	101.96	106.93
3	C	601	NDP	N3A-C2A-N1A	-3.38	123.40	128.68
2	E	600	FAD	C4X-C4-N3	3.33	121.65	113.19
3	D	601	NDP	O5B-C5B-C4B	3.32	120.40	108.99
2	A	600	FAD	C4X-C10-N10	3.27	121.27	116.48
3	C	601	NDP	PN-O3-PA	-3.25	121.66	132.83
2	C	600	FAD	C4-N3-C2	-3.23	119.68	125.64
2	A	600	FAD	O5B-C5B-C4B	-3.23	97.89	108.99
3	C	601	NDP	C2B-C3B-C4B	3.21	108.96	101.99
2	D	600	FAD	C4X-C4-N3	3.20	121.32	113.19
2	E	600	FAD	C1'-N10-C9A	-3.20	115.18	120.51
3	A	601	NDP	N3A-C2A-N1A	-3.17	123.73	128.68
2	B	600	FAD	O3'-C3'-C2'	-3.15	101.20	108.81
2	A	600	FAD	O3B-C3B-C4B	-3.13	102.01	111.05
2	B	600	FAD	C9A-C5X-N5	-3.12	119.05	122.43
2	A	600	FAD	C4-N3-C2	-3.11	119.90	125.64
3	F	601	NDP	C4A-C5A-N7A	-3.09	106.17	109.40
2	D	600	FAD	O2-C2-N1	-3.09	116.70	121.83
2	F	600	FAD	C4X-C10-N10	3.09	120.99	116.48
2	E	600	FAD	C4X-C10-N1	-3.08	117.59	124.73
2	A	600	FAD	O4'-C4'-C5'	-3.07	103.01	109.92
2	C	600	FAD	C5A-C6A-N6A	-3.06	115.70	120.35
2	F	600	FAD	C4-N3-C2	-3.04	120.02	125.64
3	B	601	NDP	O4D-C4D-C3D	3.02	107.38	104.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	600	FAD	C4A-C5A-N7A	-3.00	106.27	109.40
2	F	600	FAD	C4X-C4-N3	2.93	120.63	113.19
3	B	601	NDP	C5A-C6A-N1A	-2.88	113.81	120.35
2	B	600	FAD	C4-C4X-C10	2.87	121.62	116.79
2	C	600	FAD	C4X-C10-N10	2.85	120.64	116.48
3	E	601	NDP	C2A-N1A-C6A	2.80	123.53	118.75
3	F	601	NDP	C2A-N1A-C6A	2.79	123.53	118.75
2	D	600	FAD	C10-C4X-N5	-2.78	118.95	124.86
3	E	601	NDP	C1D-C2D-C3D	2.78	105.86	101.63
3	C	601	NDP	O4D-C4D-C3D	2.77	107.16	104.70
2	D	600	FAD	C3B-C2B-C1B	-2.76	96.82	100.98
3	A	601	NDP	O3B-C3B-C2B	-2.73	103.42	111.17
2	A	600	FAD	C9A-C5X-N5	-2.72	119.47	122.43
2	C	600	FAD	C4X-C4-N3	2.71	120.08	113.19
2	C	600	FAD	O5B-PA-O1A	2.71	119.66	109.07
2	B	600	FAD	C10-N1-C2	2.69	122.28	116.90
3	B	601	NDP	C1D-C2D-C3D	2.68	105.71	101.63
2	C	600	FAD	O4B-C4B-C3B	-2.66	99.85	105.11
2	E	600	FAD	C3B-C2B-C1B	-2.66	96.98	100.98
3	A	601	NDP	O5B-C5B-C4B	2.66	118.13	108.99
3	B	601	NDP	O5B-C5B-C4B	2.64	118.09	108.99
2	E	600	FAD	O4-C4-C4X	-2.64	119.59	126.60
2	C	600	FAD	C4X-C10-N1	-2.62	118.65	124.73
2	A	600	FAD	C10-C4X-N5	-2.59	119.36	124.86
3	B	601	NDP	O2B-C2B-C3B	2.58	121.04	111.68
2	C	600	FAD	C10-C4X-N5	-2.58	119.39	124.86
3	D	601	NDP	O2X-P2B-O2B	2.56	117.46	105.99
3	C	601	NDP	C1D-C2D-C3D	2.55	105.52	101.63
2	E	600	FAD	O2'-C2'-C3'	2.51	115.21	109.10
3	A	601	NDP	C1D-C2D-C3D	2.51	105.45	101.63
2	E	600	FAD	C6-C5X-N5	2.50	122.89	118.51
2	D	600	FAD	C5X-C9A-N10	2.49	120.53	117.95
3	F	601	NDP	C1D-C2D-C3D	2.47	105.40	101.63
2	F	600	FAD	C10-C4X-N5	-2.47	119.62	124.86
2	A	600	FAD	C5X-C9A-N10	2.46	120.50	117.95
3	C	601	NDP	O3B-C3B-C2B	-2.45	104.21	111.17
3	D	601	NDP	C1D-C2D-C3D	2.41	105.30	101.63
2	A	600	FAD	C4X-C4-N3	2.40	119.30	113.19
2	F	600	FAD	O4-C4-N3	-2.40	115.52	120.12
2	E	600	FAD	C4X-C10-N10	2.39	119.97	116.48
2	B	600	FAD	C4X-C10-N10	2.38	119.96	116.48
3	F	601	NDP	O5B-C5B-C4B	2.38	117.18	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	601	NDP	O3B-C3B-C4B	-2.36	104.22	111.05
3	D	601	NDP	N6A-C6A-N1A	2.34	123.42	118.57
2	C	600	FAD	C5X-C9A-N10	2.33	120.36	117.95
2	E	600	FAD	C10-N1-C2	2.33	121.55	116.90
3	D	601	NDP	C5A-C6A-N1A	-2.33	115.08	120.35
2	B	600	FAD	C5X-C9A-N10	2.32	120.35	117.95
3	A	601	NDP	C2A-N1A-C6A	2.32	122.73	118.75
2	E	600	FAD	O3B-C3B-C4B	-2.32	104.34	111.05
3	B	601	NDP	C4A-C5A-N7A	-2.32	106.99	109.40
2	D	600	FAD	C9A-C5X-N5	-2.30	119.93	122.43
2	C	600	FAD	PA-O5B-C5B	2.29	135.10	121.68
2	C	600	FAD	O2B-C2B-C3B	-2.26	104.52	111.82
2	B	600	FAD	C6-C5X-C9A	2.25	122.12	118.94
2	C	600	FAD	O2B-C2B-C1B	-2.21	102.71	110.85
2	A	600	FAD	O4'-C4'-C3'	2.20	114.45	109.10
2	D	600	FAD	C4X-C10-N1	-2.19	119.65	124.73
3	F	601	NDP	C5A-C6A-N1A	-2.19	115.40	120.35
2	A	600	FAD	C1'-C2'-C3'	2.18	115.88	109.79
2	D	600	FAD	O2-C2-N3	2.18	122.88	118.65
3	C	601	NDP	N6A-C6A-N1A	2.17	123.08	118.57
2	D	600	FAD	C4-C4X-N5	2.17	121.32	118.23
2	C	600	FAD	C4-C4X-C10	2.17	120.43	116.79
2	E	600	FAD	C4-C4X-C10	2.16	120.42	116.79
2	F	600	FAD	C4-C4X-N5	2.15	121.30	118.23
2	A	600	FAD	C4X-C10-N1	-2.14	119.76	124.73
2	B	600	FAD	C3B-C2B-C1B	-2.14	97.76	100.98
2	E	600	FAD	N6A-C6A-N1A	-2.13	114.14	118.57
3	D	601	NDP	O5B-PA-O1A	2.13	117.39	109.07
2	D	600	FAD	O2B-C2B-C1B	-2.12	103.01	110.85
2	E	600	FAD	C9A-N10-C10	-2.12	117.47	120.77
2	A	600	FAD	C4-C4X-C10	2.10	120.33	116.79
3	C	601	NDP	O4B-C1B-C2B	-2.10	102.94	106.59
2	D	600	FAD	O4-C4-C4X	-2.08	121.07	126.60
3	F	601	NDP	N6A-C6A-N1A	2.08	122.90	118.57
2	C	600	FAD	C5B-C4B-C3B	2.08	122.98	115.18
2	B	600	FAD	O2'-C2'-C3'	2.07	114.13	109.10
2	B	600	FAD	N6A-C6A-N1A	-2.04	114.35	118.57
3	B	601	NDP	C5A-C6A-N6A	2.03	123.44	120.35
3	A	601	NDP	O4B-C4B-C5B	-2.03	102.71	109.37
2	F	600	FAD	O4'-C4'-C3'	2.01	113.98	109.10
3	B	601	NDP	N6A-C6A-N1A	2.00	122.73	118.57

There are no chirality outliers.

All (97) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C5'-O5'-P-O2P
2	C	600	FAD	C3B-C4B-C5B-O5B
2	C	600	FAD	N10-C1'-C2'-O2'
2	C	600	FAD	N10-C1'-C2'-C3'
2	C	600	FAD	C2'-C3'-C4'-O4'
2	C	600	FAD	C2'-C3'-C4'-C5'
2	C	600	FAD	O3'-C3'-C4'-O4'
2	D	600	FAD	O4B-C4B-C5B-O5B
2	D	600	FAD	PA-O3P-P-O5'
2	E	600	FAD	O4B-C4B-C5B-O5B
2	E	600	FAD	C5'-O5'-P-O2P
2	F	600	FAD	O4B-C4B-C5B-O5B
2	F	600	FAD	C2'-C3'-C4'-O4'
2	F	600	FAD	O3'-C3'-C4'-O4'
2	F	600	FAD	O3'-C3'-C4'-C5'
2	F	600	FAD	PA-O3P-P-O5'
3	A	601	NDP	C5D-O5D-PN-O3
3	A	601	NDP	C5D-O5D-PN-O1N
3	A	601	NDP	C5D-O5D-PN-O2N
3	A	601	NDP	O4D-C4D-C5D-O5D
3	A	601	NDP	C3D-C4D-C5D-O5D
3	C	601	NDP	O4B-C4B-C5B-O5B
3	C	601	NDP	PA-O3-PN-O5D
3	D	601	NDP	C5B-O5B-PA-O3
3	D	601	NDP	C5D-O5D-PN-O3
3	D	601	NDP	C5D-O5D-PN-O2N
3	F	601	NDP	C5D-O5D-PN-O1N
3	F	601	NDP	C5D-O5D-PN-O2N
2	A	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
2	D	600	FAD	C3B-C4B-C5B-O5B
2	F	600	FAD	C3B-C4B-C5B-O5B
3	B	601	NDP	O4D-C4D-C5D-O5D
3	B	601	NDP	C3D-C4D-C5D-O5D
3	C	601	NDP	C3B-C4B-C5B-O5B
3	E	601	NDP	O4B-C4B-C5B-O5B
3	E	601	NDP	C3B-C4B-C5B-O5B
3	E	601	NDP	O4D-C4D-C5D-O5D
3	E	601	NDP	C3D-C4D-C5D-O5D
3	E	601	NDP	C4D-C5D-O5D-PN

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Mol	Chain	Res	Type	Atoms
2	C	600	FAD	O3'-C3'-C4'-C5'
2	F	600	FAD	C2'-C3'-C4'-C5'
2	A	600	FAD	C3B-C4B-C5B-O5B
2	E	600	FAD	C3B-C4B-C5B-O5B
3	D	601	NDP	O4B-C4B-C5B-O5B
3	D	601	NDP	C3B-C4B-C5B-O5B
2	C	600	FAD	O4B-C4B-C5B-O5B
3	D	601	NDP	C4B-C5B-O5B-PA
2	A	600	FAD	PA-O3P-P-O5'
2	E	600	FAD	PA-O3P-P-O5'
3	A	601	NDP	PN-O3-PA-O5B
3	F	601	NDP	PA-O3-PN-O5D
3	F	601	NDP	C2B-O2B-P2B-O1X
3	B	601	NDP	C4D-C5D-O5D-PN
2	A	600	FAD	C5'-O5'-P-O3P
2	C	600	FAD	C5B-O5B-PA-O3P
2	F	600	FAD	C5'-O5'-P-O3P
2	E	600	FAD	P-O3P-PA-O2A
3	B	601	NDP	PA-O3-PN-O1N
3	D	601	NDP	PN-O3-PA-O2A
3	C	601	NDP	C4B-C5B-O5B-PA
2	A	600	FAD	C5'-O5'-P-O1P
2	C	600	FAD	C5B-O5B-PA-O2A
2	E	600	FAD	C5'-O5'-P-O1P
2	F	600	FAD	C5'-O5'-P-O1P
2	F	600	FAD	C5'-O5'-P-O2P
3	D	601	NDP	C5B-O5B-PA-O1A
3	D	601	NDP	C5D-O5D-PN-O1N
2	A	600	FAD	P-O3P-PA-O2A
2	D	600	FAD	P-O3P-PA-O2A
3	B	601	NDP	C4B-C5B-O5B-PA
3	A	601	NDP	C4B-C5B-O5B-PA
2	E	600	FAD	C2'-C1'-N10-C10
3	A	601	NDP	PA-O3-PN-O1N
3	B	601	NDP	PA-O3-PN-O2N
3	A	601	NDP	C3B-C4B-C5B-O5B
3	A	601	NDP	C2B-O2B-P2B-O1X
2	B	600	FAD	C5B-O5B-PA-O3P
3	A	601	NDP	C2B-O2B-P2B-O3X
3	B	601	NDP	C2B-O2B-P2B-O3X
3	C	601	NDP	C5D-O5D-PN-O3
3	D	601	NDP	C2B-O2B-P2B-O3X

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Mol	Chain	Res	Type	Atoms
3	F	601	NDP	C5D-O5D-PN-O3
3	A	601	NDP	O4B-C4B-C5B-O5B
3	D	601	NDP	O4D-C4D-C5D-O5D
2	A	600	FAD	P-O3P-PA-O1A
2	D	600	FAD	P-O3P-PA-O1A
2	E	600	FAD	P-O3P-PA-O1A
2	E	600	FAD	PA-O3P-P-O2P
3	D	601	NDP	PN-O3-PA-O1A
3	A	601	NDP	C5B-O5B-PA-O1A
3	B	601	NDP	C5B-O5B-PA-O1A
3	B	601	NDP	O4B-C4B-C5B-O5B
3	F	601	NDP	O4B-C4B-C5B-O5B
2	E	600	FAD	O4'-C4'-C5'-O5'

There are no ring outliers.

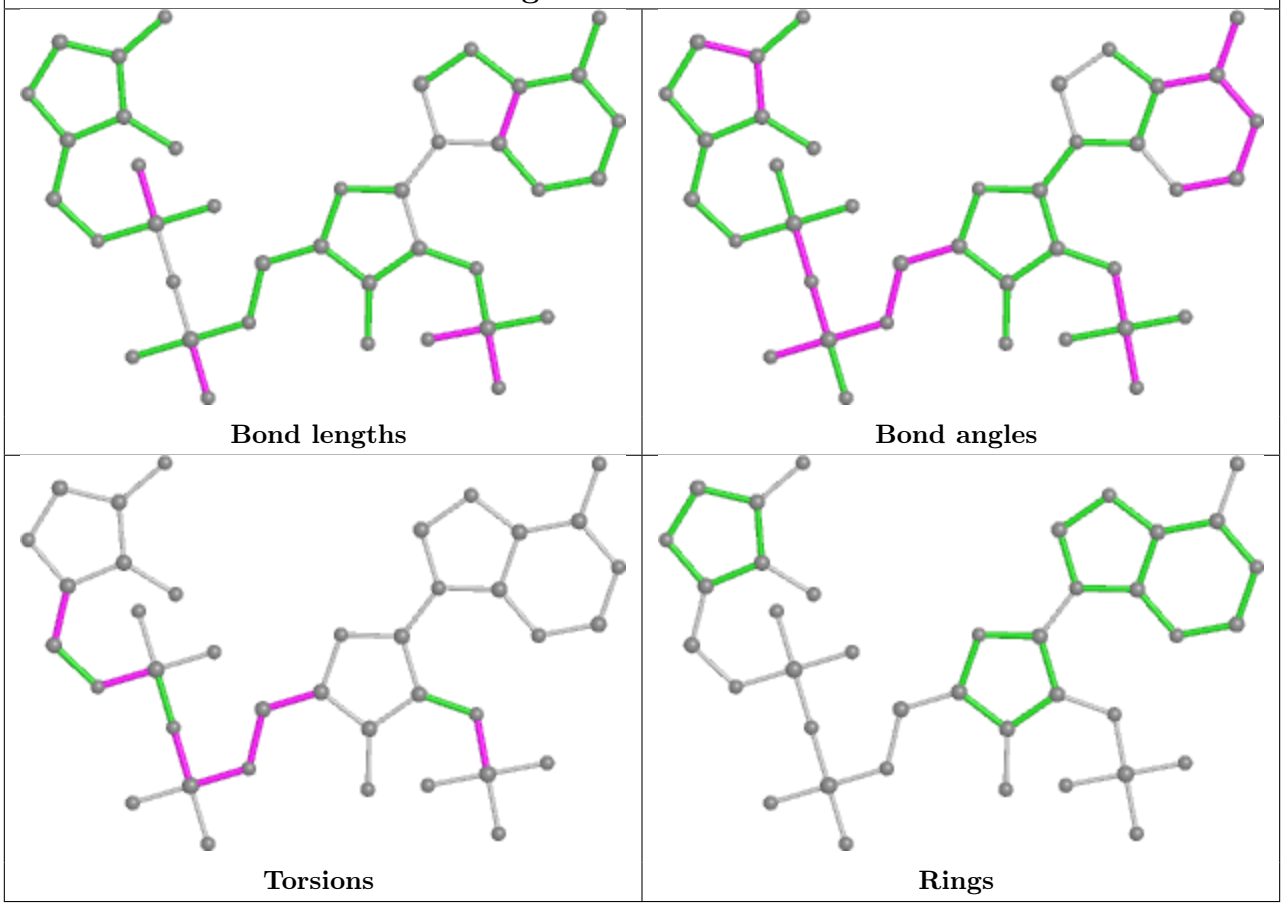
12 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	FAD	4	0
2	E	600	FAD	3	0
3	B	601	NDP	8	0
3	C	601	NDP	6	0
2	C	600	FAD	17	0
2	B	600	FAD	10	0
3	A	601	NDP	2	0
3	E	601	NDP	1	0
3	D	601	NDP	6	0
2	F	600	FAD	5	0
3	F	601	NDP	4	0
2	A	600	FAD	5	0

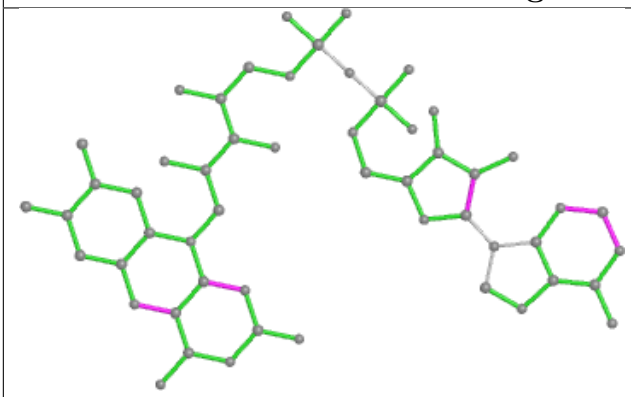
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.

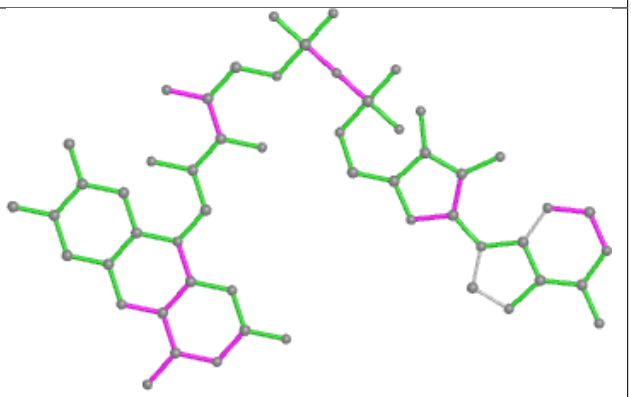
Ligand NDP D 601



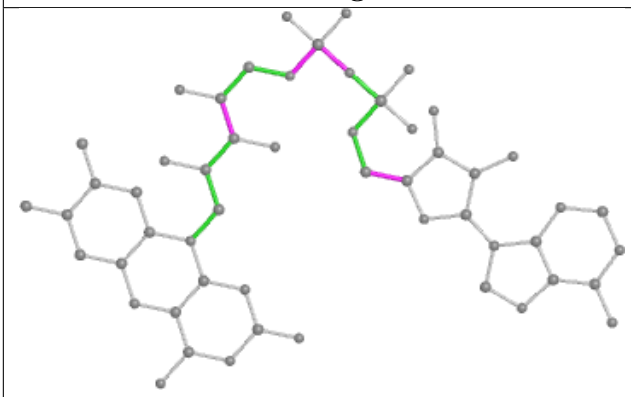
Ligand FAD F 600



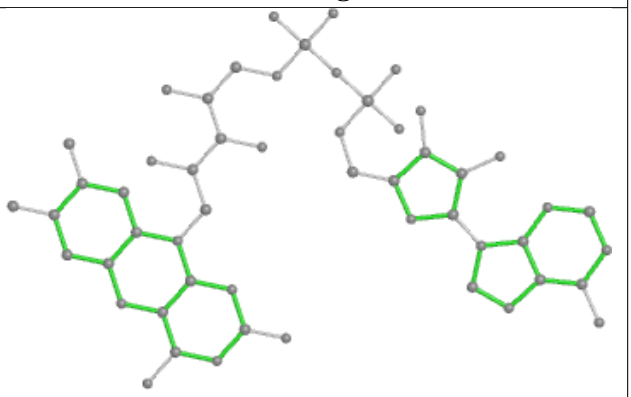
Bond lengths



Bond angles

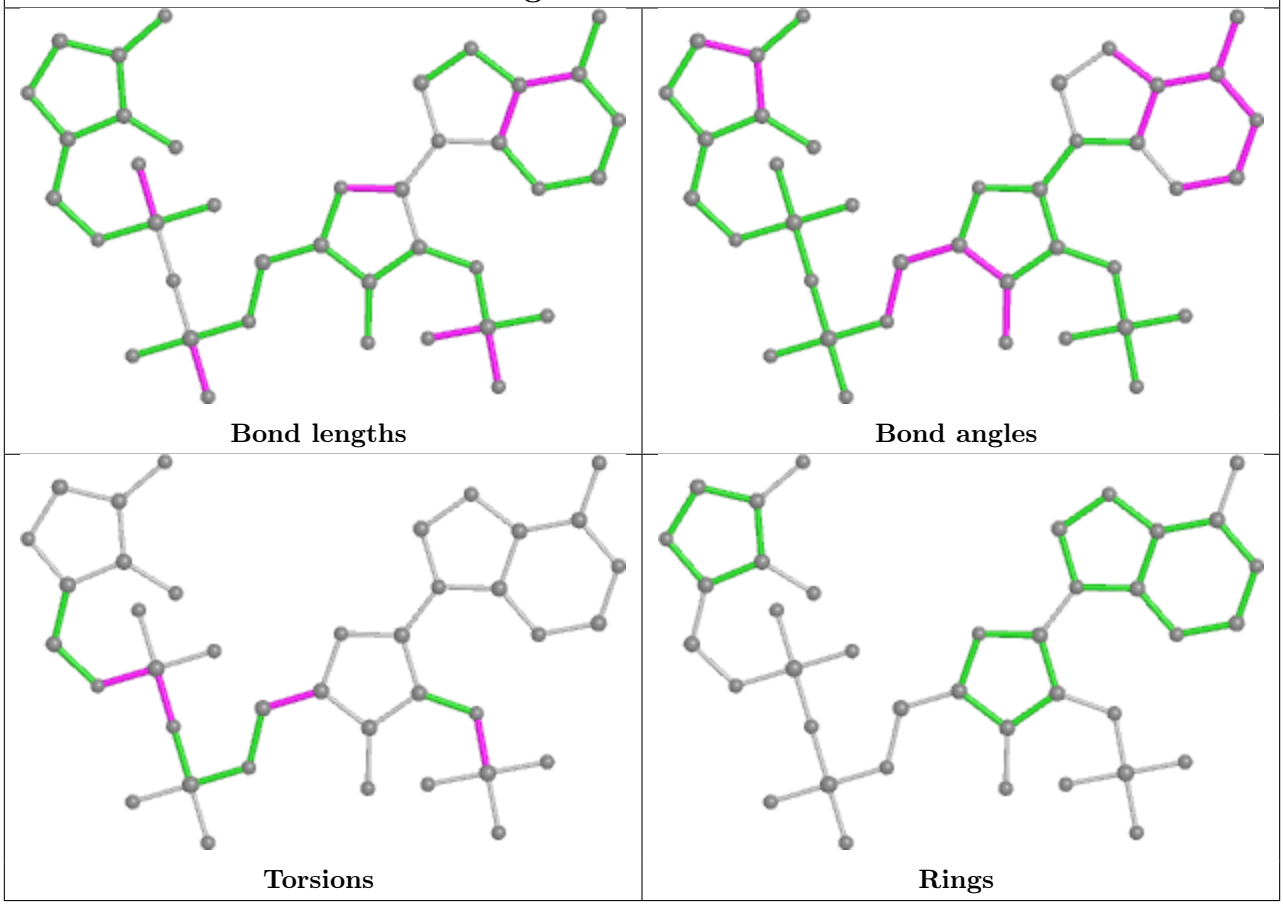


Torsions



Rings

Ligand NDP F 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	490/499 (98%)	-0.38	2 (0%)	92	79	7, 13, 20, 48	0
1	B	487/499 (97%)	-0.48	1 (0%)	95	87	6, 13, 20, 39	0
1	C	482/499 (96%)	0.11	16 (3%)	46	20	6, 13, 19, 44	0
1	D	487/499 (97%)	-0.33	4 (0%)	86	65	6, 12, 19, 38	0
1	E	491/499 (98%)	-0.39	4 (0%)	86	65	7, 13, 20, 48	0
1	F	490/499 (98%)	-0.24	6 (1%)	79	54	6, 13, 20, 48	0
All	All	2927/2994 (97%)	-0.29	33 (1%)	80	56	6, 13, 20, 48	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	497	CYS	6.9
1	E	495	SER	5.5
1	C	297	THR	5.1
1	F	495	SER	5.1
1	A	498	CYS	3.6
1	C	306	GLY	3.6
1	D	494	GLN	3.3
1	A	497	CYS	3.1
1	F	498	CYS	3.1
1	E	498	CYS	3.0
1	C	35	ASP	2.9
1	D	495	SER	2.8
1	C	296	CYS	2.8
1	E	496	GLY	2.8
1	C	256	ILE	2.6
1	C	135	ILE	2.6
1	C	275	ASN	2.6
1	F	494	GLN	2.5
1	C	335	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	134	PHE	2.3
1	C	361	SER	2.3
1	F	297	THR	2.2
1	C	182	ASP	2.2
1	F	496	GLY	2.2
1	D	394	PHE	2.2
1	C	250	GLN	2.2
1	C	257	GLU	2.2
1	B	494	GLN	2.2
1	F	499	GLY	2.1
1	D	114	TRP	2.1
1	C	298	ARG	2.0
1	C	281	GLU	2.0
1	C	168	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NDP	C	601	39/48	0.77	0.26	82,92,100,101	0
3	NDP	F	601	39/48	0.78	0.29	72,95,112,112	0
3	NDP	D	601	39/48	0.85	0.20	44,55,77,77	0
3	NDP	A	601	39/48	0.85	0.22	41,49,78,78	0
2	FAD	C	600	53/53	0.86	0.28	34,45,49,51	0
3	NDP	B	601	39/48	0.89	0.22	31,50,69,71	0
3	NDP	E	601	39/48	0.91	0.21	45,52,76,79	0
2	FAD	F	600	53/53	0.92	0.26	27,33,53,55	0
2	FAD	E	600	53/53	0.94	0.28	10,17,54,56	0

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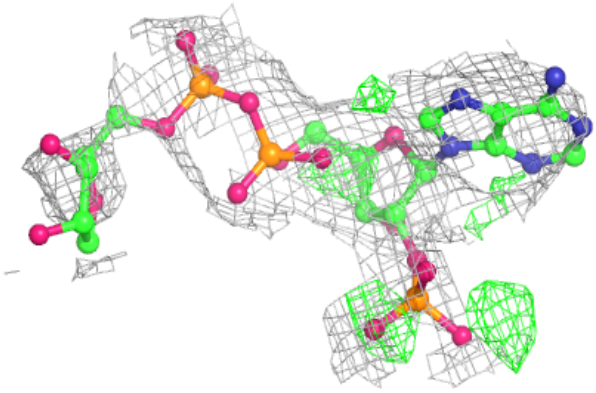
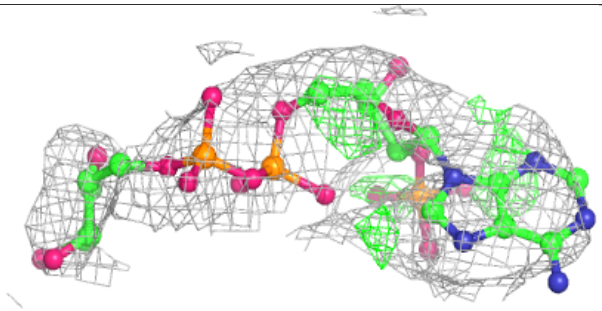
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FAD	A	600	53/53	0.94	0.22	14,24,36,36	0
2	FAD	B	600	53/53	0.95	0.25	18,26,42,46	0
2	FAD	D	600	53/53	0.95	0.29	20,29,40,47	0

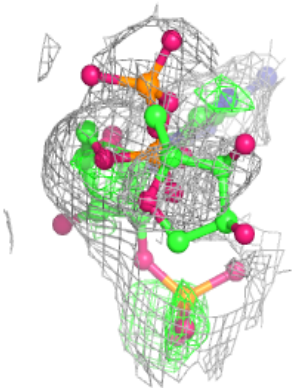
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NDP C 601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

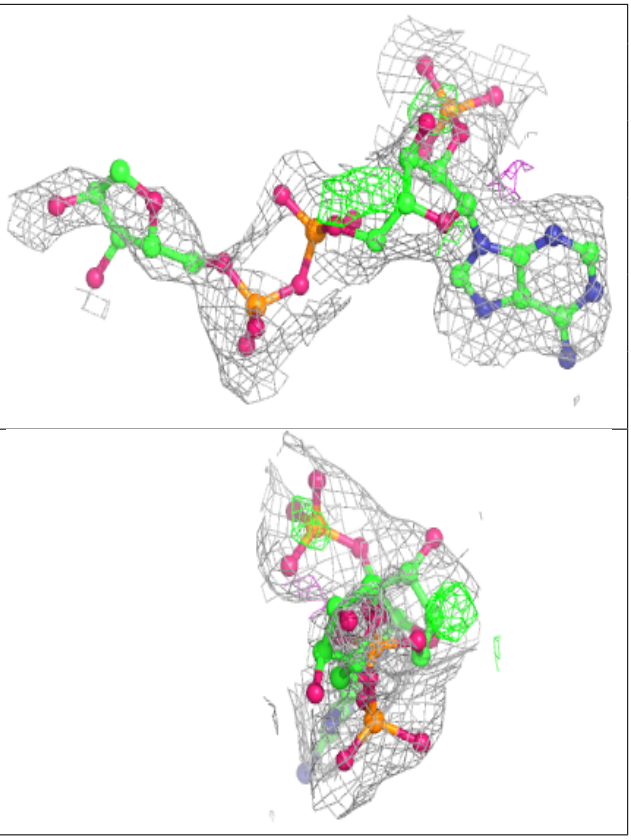


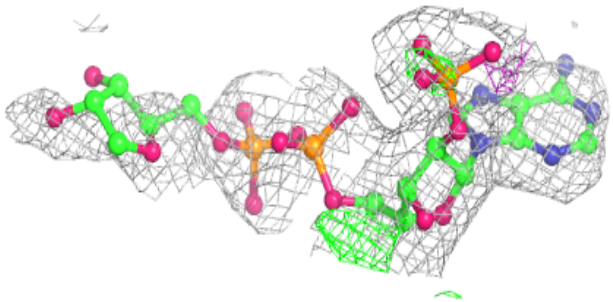




Electron density around NDP F 601:

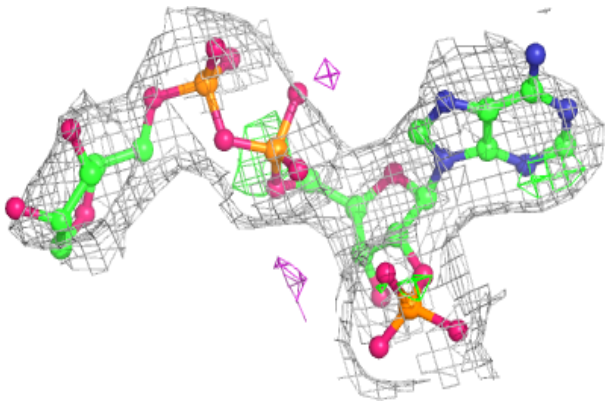
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

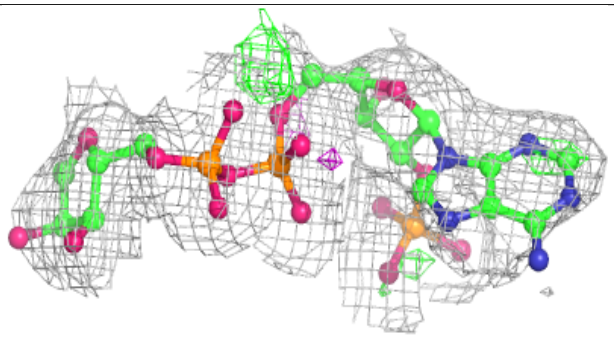


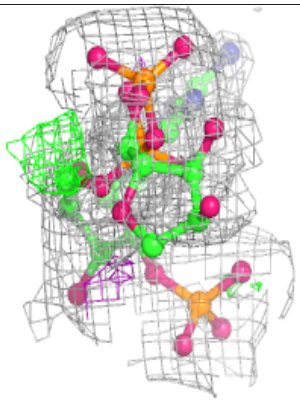


Electron density around NDP D 601:

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

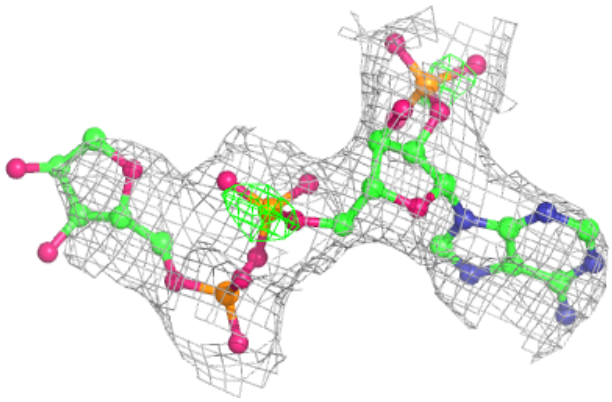


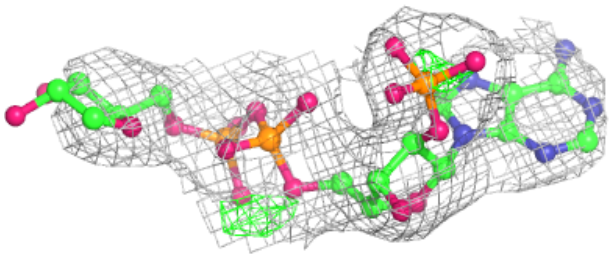


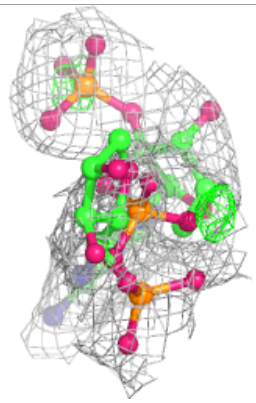


Electron density around NDP A 601:

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

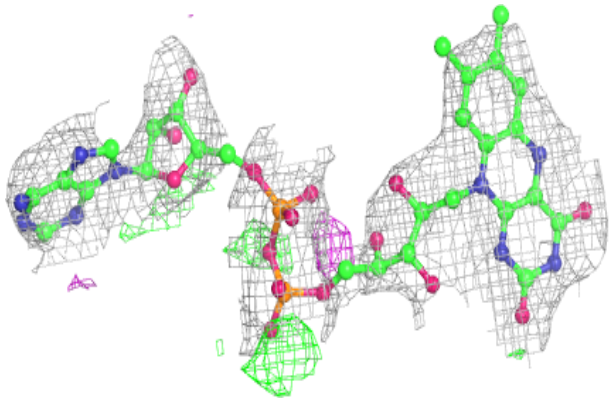


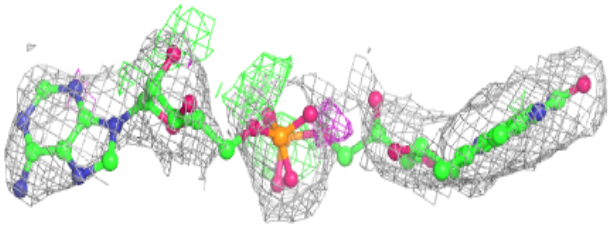




Electron density around FAD C 600:

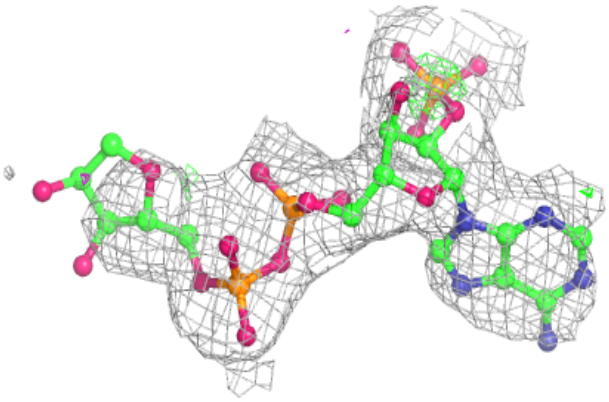
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

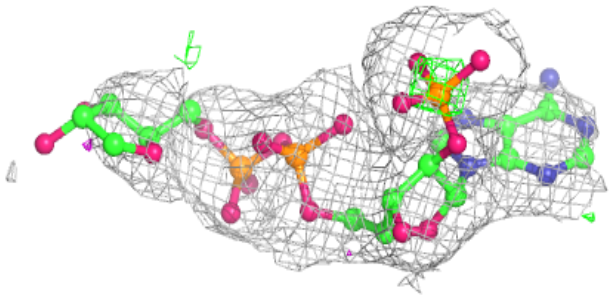


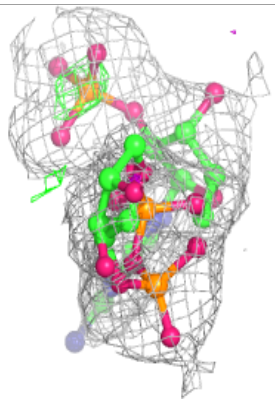


Electron density around NDP B 601:

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

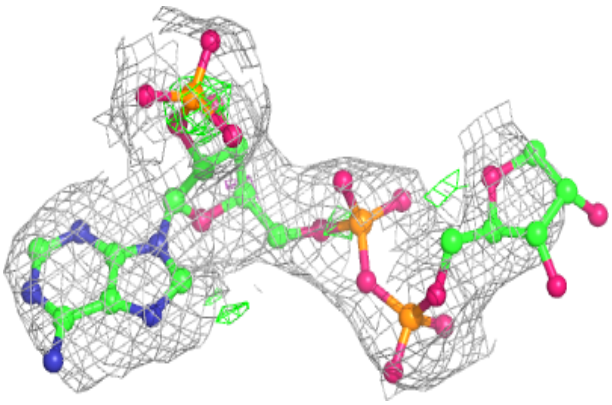


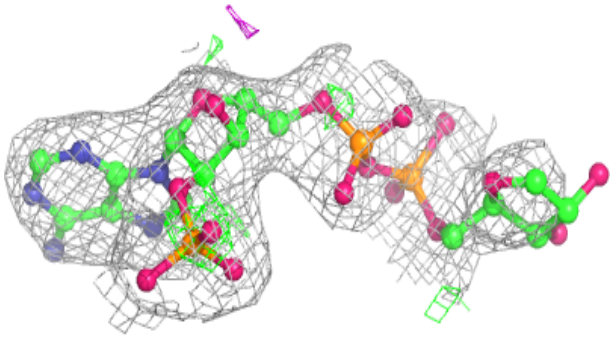


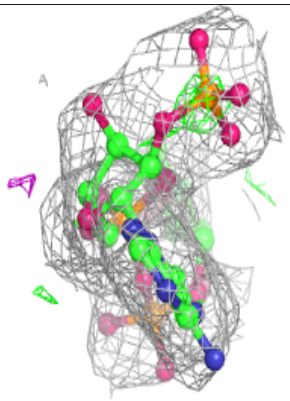


Electron density around NDP E 601:

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

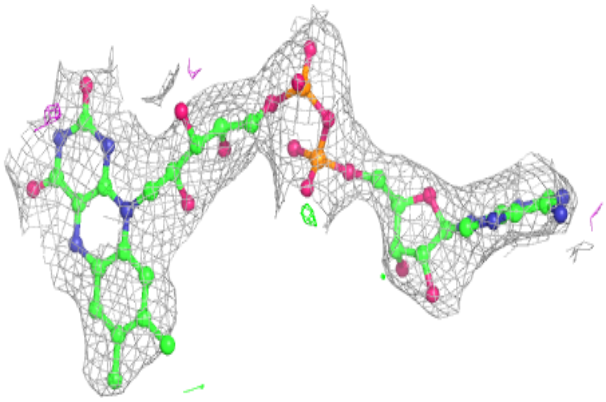


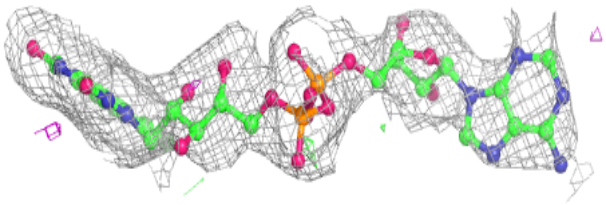


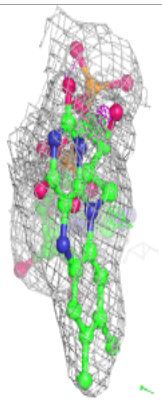


Electron density around FAD F 600:

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

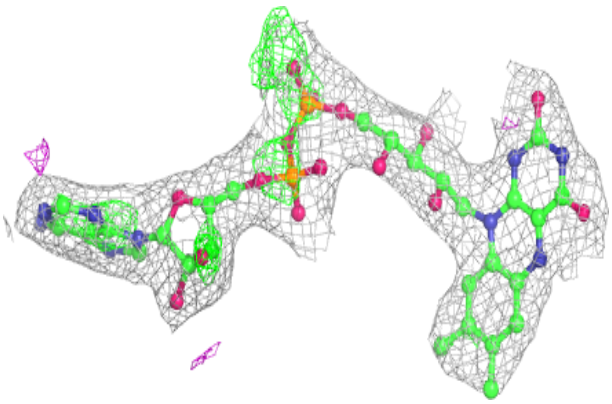


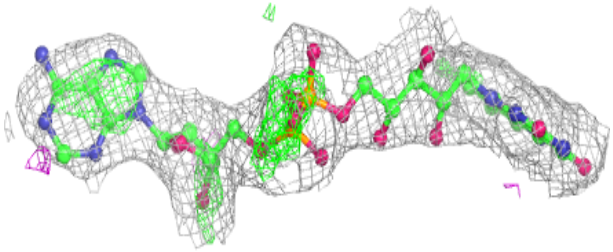


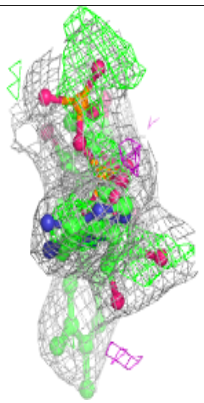


Electron density around FAD E 600:

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

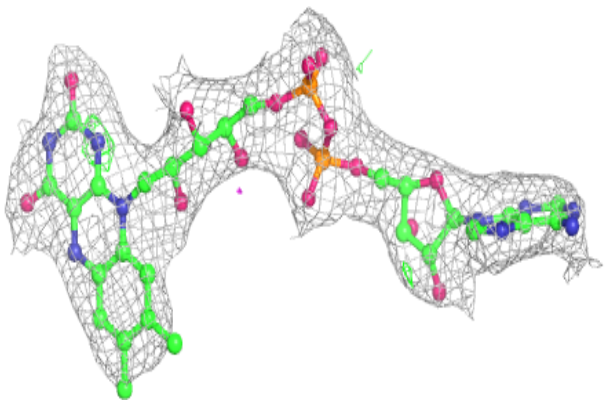


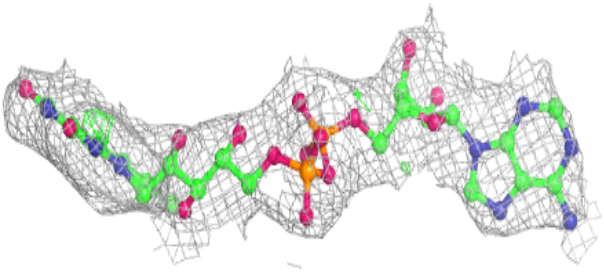


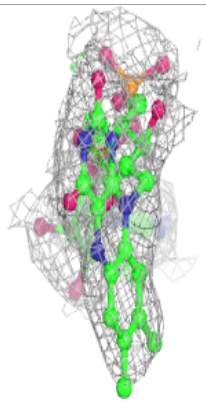


Electron density around FAD A 600:

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

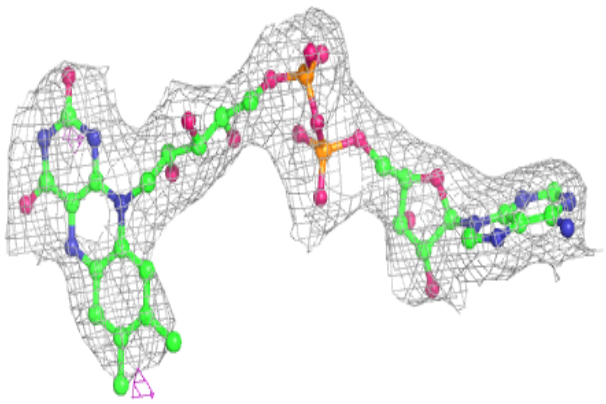


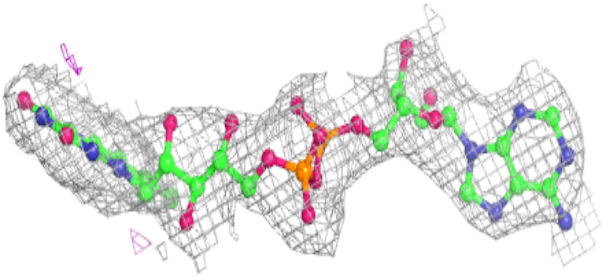


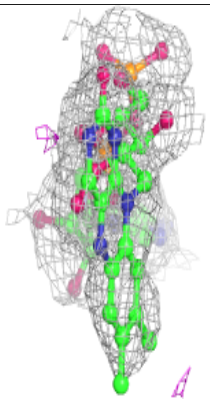


Electron density around FAD B 600:

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

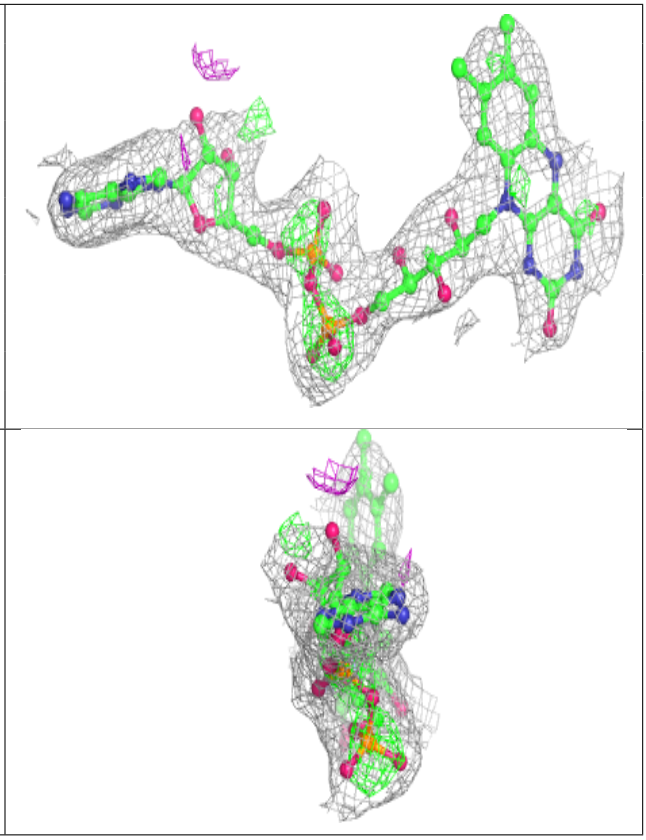






Electron density around FAD D 600:

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



6.5 Other polymers (i)

There are no such residues in this entry.