



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2024 – 12:54 PM JST

PDB ID : 8J2S
Title : Glucosyl transferase NbUGT72AY1 co-crystallized with Scopoletin, UDP-2F
Glucose and Retinol
Authors : Hameed, U.F.S.; Arold, S.T.
Deposited on : 2023-04-15
Resolution : 3.26 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (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

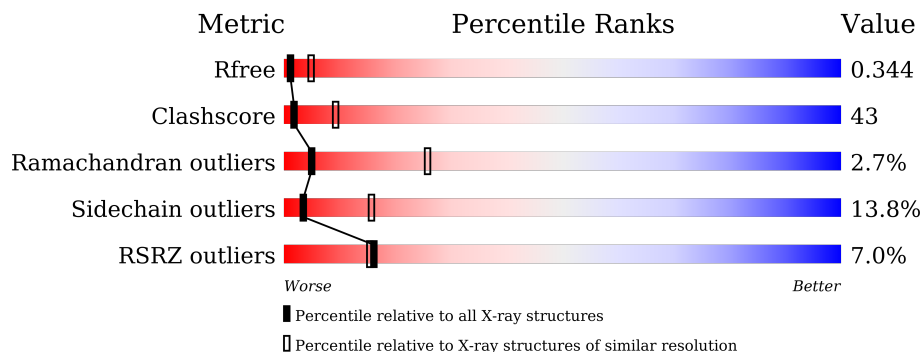
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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

Mol	Chain	Length	Quality of chain
1	A	482	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 44%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">5% 44% 38% 12% • 5%</p>
1	B	482	<div style="display: flex; align-items: center;"> <div style="width: 4%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 48%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">4% 48% 40% 7% • 5%</p>
1	C	482	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 45%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 40%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">6% 45% 40% 9% • 5%</p>
1	D	482	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 38%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">5% 46% 38% 10% • 5%</p>
1	E	482	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 43%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 41%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">8% 43% 41% 10% • 5%</p>
1	F	482	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 46%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 39%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 10%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: grey; margin-right: 5px;"></div> </div> <p style="margin-left: 5px;">6% 46% 39% 10% • 5%</p>

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Mol	Chain	Length	Quality of chain
1	G	482	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	U2F	A	501	-	-	X	-
2	U2F	C	501	-	-	X	-
2	U2F	D	501	-	-	X	-
2	U2F	E	501	-	-	X	-
2	U2F	G	501	-	-	X	-
3	T83	A	502	-	X	-	-
3	T83	B	502	-	X	-	-
3	T83	C	502	-	X	-	-
3	T83	D	502	-	X	-	-
3	T83	F	502	-	X	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 25774 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 Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	458	3627	2318	610	683	16	0	0	0
1	B	460	3640	2325	612	687	16	0	0	0
1	C	460	3640	2325	612	687	16	0	0	0
1	D	459	3633	2321	611	685	16	0	0	0
1	E	459	3632	2319	611	686	16	0	0	0
1	F	460	3640	2325	612	687	16	0	0	0
1	G	460	3640	2325	612	687	16	0	0	0

There are 35 discrepancies between the modelled and reference sequences:

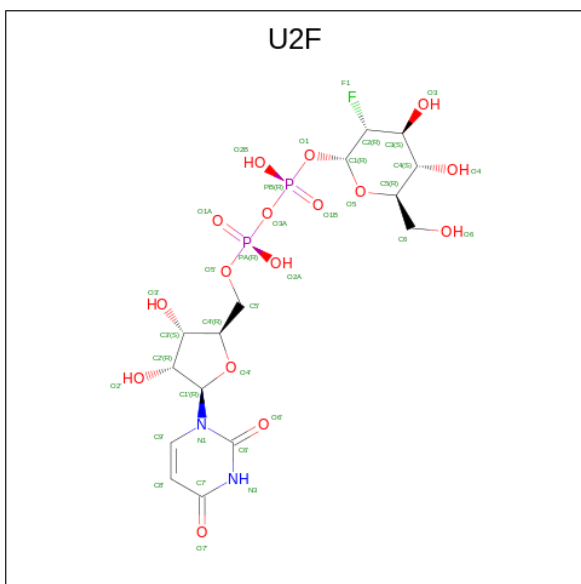
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
A	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
A	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
A	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
A	0	SER	-	expression tag	UNP A0A8K1ZRH3
B	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
B	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
B	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
B	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
B	0	SER	-	expression tag	UNP A0A8K1ZRH3
C	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
C	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
C	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
C	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
C	0	SER	-	expression tag	UNP A0A8K1ZRH3

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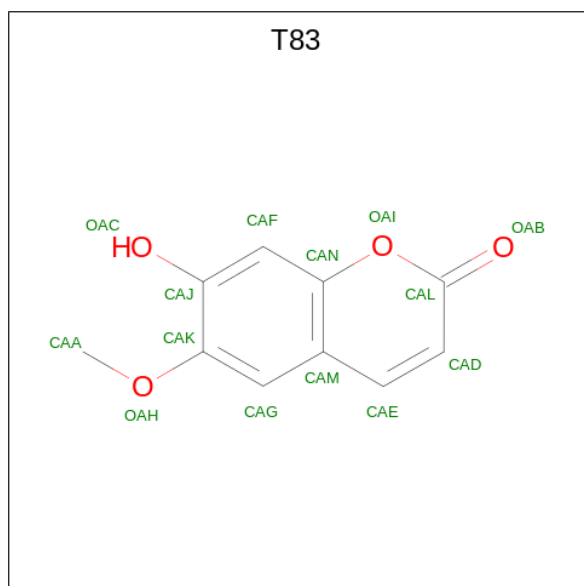
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
D	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
D	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
D	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
D	0	SER	-	expression tag	UNP A0A8K1ZRH3
E	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
E	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
E	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
E	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
E	0	SER	-	expression tag	UNP A0A8K1ZRH3
F	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
F	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
F	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
F	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
F	0	SER	-	expression tag	UNP A0A8K1ZRH3
G	-4	GLY	-	expression tag	UNP A0A8K1ZRH3
G	-3	PRO	-	expression tag	UNP A0A8K1ZRH3
G	-2	LEU	-	expression tag	UNP A0A8K1ZRH3
G	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
G	0	SER	-	expression tag	UNP A0A8K1ZRH3

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-2-DEOXY-2-FLUORO-ALPHA-D-GLUCOSE (three-letter code: U2F) (formula: C₁₅H₂₃FN₂O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	B	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	C	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	D	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	E	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	F	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	G	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		

- Molecule 3 is 7-hydroxy-6-methoxy-2H-1-benzopyran-2-one (three-letter code: T83) (formula: C₁₀H₈O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	C O	0	0
			14	10 4		
3	B	1	Total	C O	0	0
			14	10 4		
3	C	1	Total	C O	0	0
			14	10 4		
3	D	1	Total	C O	0	0
			14	10 4		

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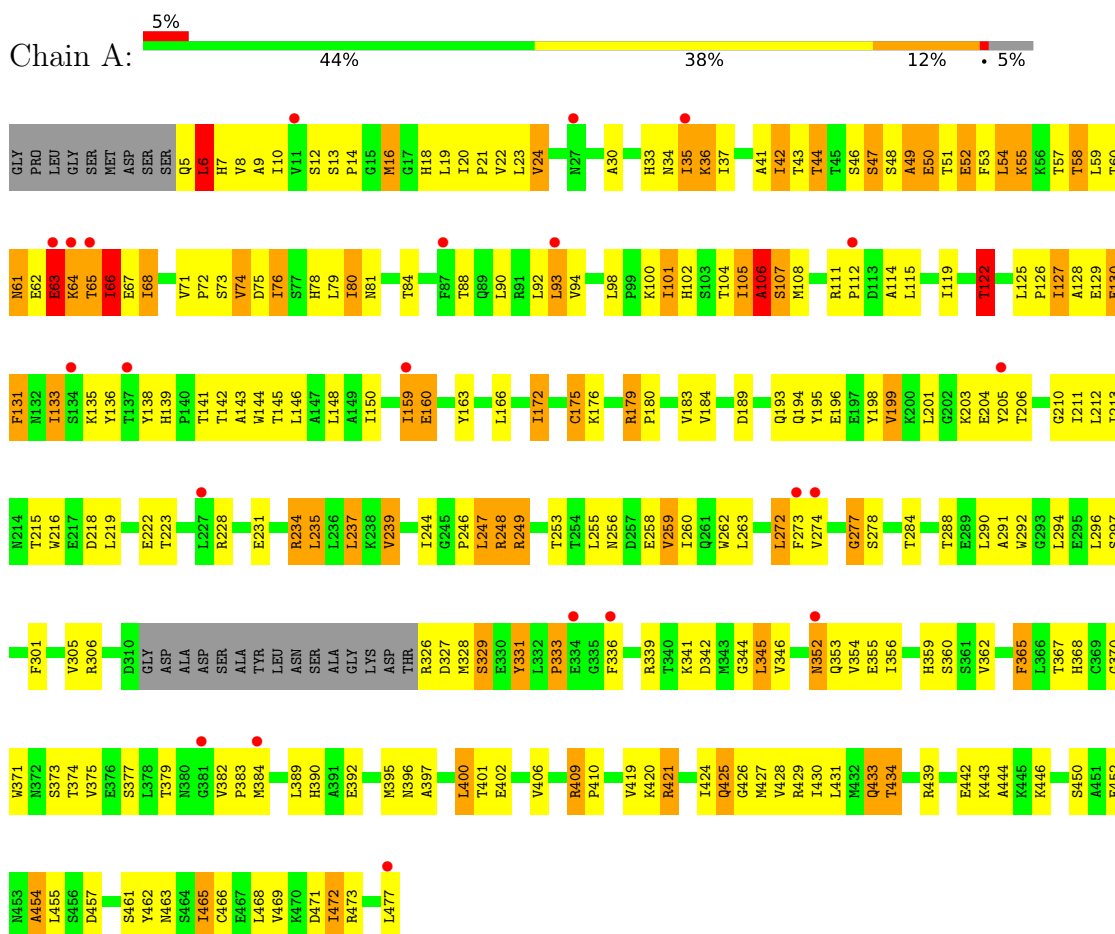
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	F	1	14	10	4	0	0

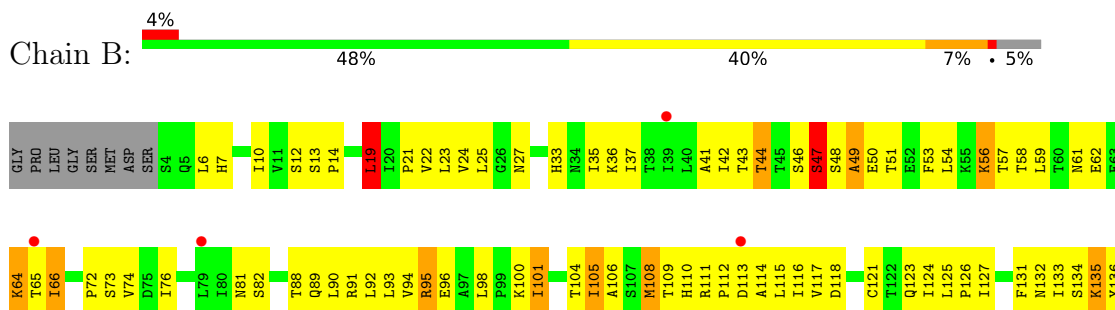
3 Residue-property plots i

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: Glycosyltransferase

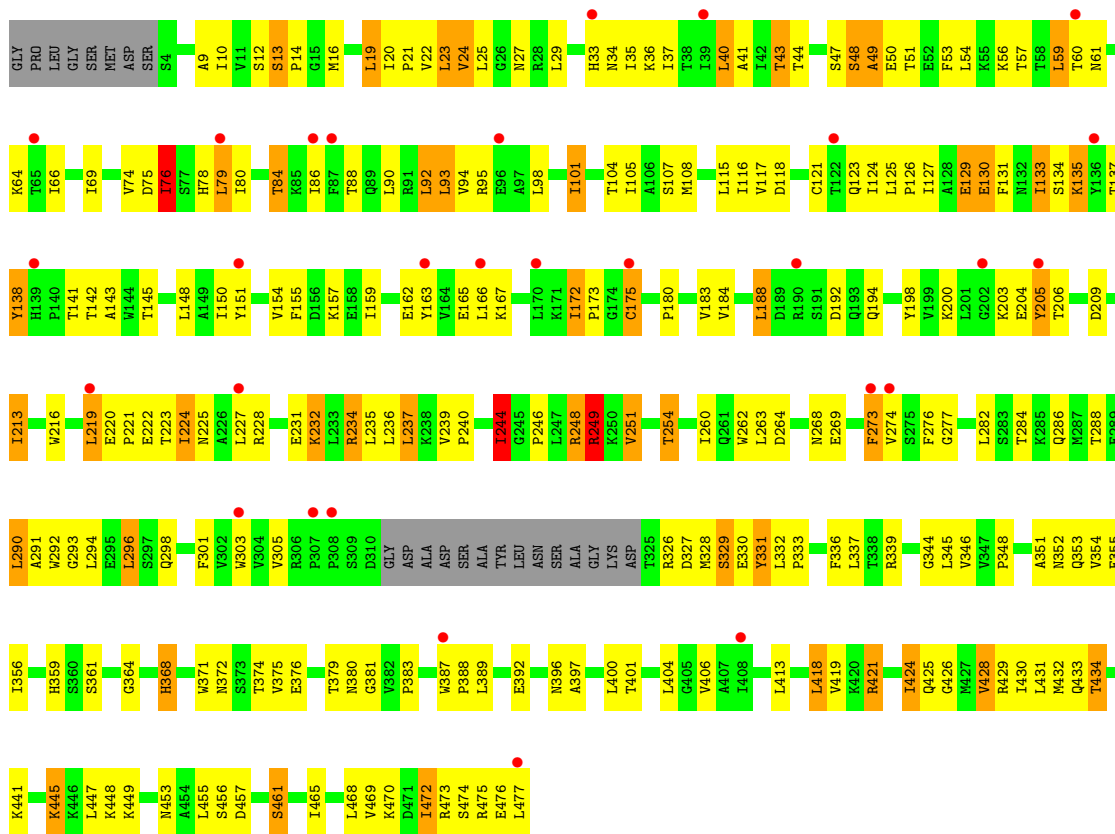


- Molecule 1: Glycosyltransferase

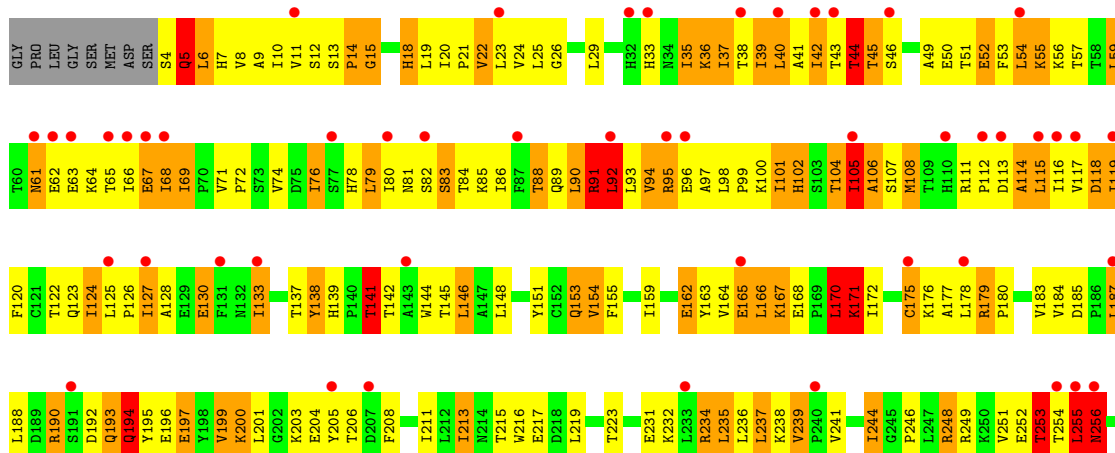


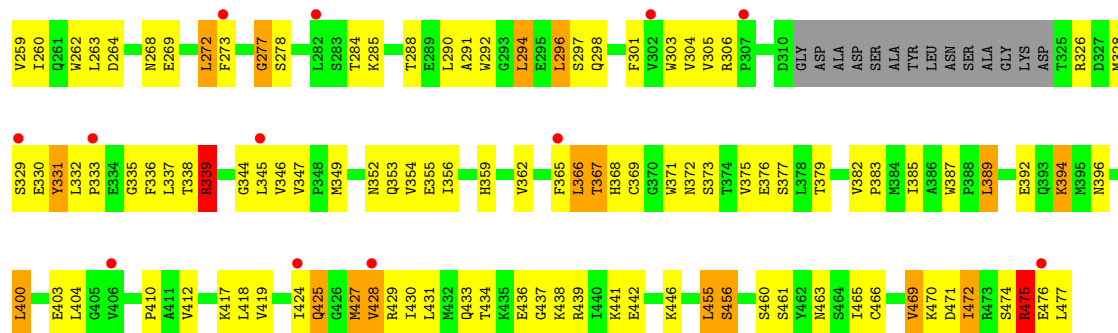


• Molecule 1: Glycosyltransferase



• Molecule 1: Glycosyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.13Å 170.39Å 152.13Å 90.00° 93.39° 90.00°	Depositor
Resolution (Å)	48.57 – 3.26 48.53 – 3.26	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.57-3.26) 83.8 (48.53-3.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.25Å)	Xtrriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.303 , 0.342 0.303 , 0.344	Depositor DCC
R_{free} test set	3300 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	96.2	Xtrriage
Anisotropy	0.663	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	25774	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: T83, U2F

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	0.51	1/3698 (0.0%)	0.80	3/5016 (0.1%)
1	B	0.53	2/3711 (0.1%)	0.75	3/5034 (0.1%)
1	C	0.51	3/3711 (0.1%)	0.77	2/5034 (0.0%)
1	D	0.49	0/3703	0.76	4/5021 (0.1%)
1	E	0.52	1/3702 (0.0%)	0.81	3/5020 (0.1%)
1	F	0.49	1/3711 (0.0%)	0.81	5/5034 (0.1%)
1	G	0.57	1/3711 (0.0%)	0.88	6/5034 (0.1%)
All	All	0.52	9/25947 (0.0%)	0.80	26/35193 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	B	0	7
1	C	0	6
1	D	0	8
1	E	0	9
1	F	0	6
1	G	0	13
All	All	0	58

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	440	ILE	CG1-CD1	-8.44	0.92	1.50
1	C	150	ILE	CG1-CD1	-7.32	0.99	1.50
1	G	427	MET	SD-CE	-6.00	1.44	1.77
1	B	150	ILE	CG1-CD1	-5.91	1.09	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	432	MET	SD-CE	-5.71	1.45	1.77
1	C	42	ILE	CG1-CD1	-5.44	1.12	1.50
1	A	122	THR	CB-CG2	5.22	1.69	1.52
1	F	213	ILE	CG1-CD1	-5.11	1.15	1.50
1	C	37	ILE	CG1-CD1	-5.01	1.15	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	159	ILE	CB-CA-C	-15.49	80.62	111.60
1	E	159	ILE	N-CA-C	10.58	139.56	111.00
1	D	262	TRP	N-CA-C	-9.32	85.84	111.00
1	F	269	GLU	CB-CA-C	7.96	126.31	110.40
1	G	105	ILE	N-CA-C	-7.45	90.89	111.00
1	F	269	GLU	N-CA-C	-7.31	91.27	111.00
1	G	170	LEU	N-CA-C	7.23	130.52	111.00
1	C	123	GLN	N-CA-C	-6.95	92.23	111.00
1	F	130	GLU	N-CA-C	-6.67	93.00	111.00
1	B	213	ILE	N-CA-C	6.58	128.78	111.00
1	A	130	GLU	N-CA-C	-6.55	93.32	111.00
1	G	105	ILE	N-CA-CB	6.46	125.65	110.80
1	A	454	ALA	N-CA-C	-5.99	94.82	111.00
1	F	244	ILE	N-CA-C	-5.90	95.06	111.00
1	D	454	ALA	N-CA-C	-5.83	95.26	111.00
1	G	455	LEU	N-CA-C	-5.79	95.36	111.00
1	D	262	TRP	CB-CA-C	5.77	121.94	110.40
1	B	431	LEU	N-CA-C	-5.61	95.86	111.00
1	G	92	LEU	CA-CB-CG	5.57	128.11	115.30
1	D	386	ALA	N-CA-C	5.52	125.91	111.00
1	B	19	LEU	CB-CG-CD1	5.51	120.37	111.00
1	E	431	LEU	N-CA-C	-5.51	96.11	111.00
1	F	368	HIS	CB-CG-ND1	-5.31	109.92	123.20
1	G	141	THR	CA-CB-OG1	5.28	120.08	109.00
1	C	54	LEU	CB-CA-C	-5.24	100.25	110.20
1	A	63	GLU	N-CA-C	5.18	124.98	111.00

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	ALA	Peptide
1	A	179	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	234	ARG	Sidechain
1	A	248	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	339	ARG	Sidechain
1	A	409	ARG	Sidechain
1	A	421	ARG	Sidechain
1	A	63	GLU	Peptide
1	B	190	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	339	ARG	Sidechain
1	B	381	GLY	Peptide
1	B	473	ARG	Sidechain
1	B	91	ARG	Sidechain
1	B	95	ARG	Sidechain
1	C	179	ARG	Sidechain
1	C	326	ARG	Sidechain
1	C	381	GLY	Peptide
1	C	421	ARG	Sidechain
1	C	91	ARG	Sidechain
1	C	95	ARG	Sidechain
1	D	111	ARG	Sidechain
1	D	179	ARG	Sidechain
1	D	248	ARG	Sidechain
1	D	249	ARG	Sidechain
1	D	262	TRP	Mainchain
1	D	326	ARG	Sidechain
1	D	381	GLY	Peptide
1	D	95	ARG	Sidechain
1	E	111	ARG	Sidechain
1	E	159	ILE	Peptide
1	E	190	ARG	Sidechain
1	E	234	ARG	Sidechain
1	E	248	ARG	Sidechain
1	E	28	ARG	Sidechain
1	E	381	GLY	Peptide
1	E	421	ARG	Sidechain
1	E	91	ARG	Sidechain
1	F	234	ARG	Sidechain
1	F	248	ARG	Sidechain
1	F	249	ARG	Sidechain
1	F	339	ARG	Sidechain
1	F	421	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	473	ARG	Sidechain
1	G	104	THR	Peptide
1	G	106	ALA	Peptide
1	G	179	ARG	Sidechain
1	G	234	ARG	Sidechain
1	G	248	ARG	Sidechain
1	G	253	THR	Peptide
1	G	256	ASN	Peptide
1	G	339	ARG	Sidechain
1	G	44	THR	Peptide
1	G	475	ARG	Sidechain
1	G	5	GLN	Peptide
1	G	83	SER	Peptide
1	G	91	ARG	Sidechain

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	3627	0	3718	304	0
1	B	3640	0	3730	263	0
1	C	3640	0	3730	322	0
1	D	3633	0	3722	253	0
1	E	3632	0	3718	313	0
1	F	3640	0	3730	286	0
1	G	3640	0	3730	507	0
2	A	36	0	21	11	0
2	B	36	0	21	8	0
2	C	36	0	21	36	0
2	D	36	0	21	11	0
2	E	36	0	21	15	0
2	F	36	0	21	7	0
2	G	36	0	21	9	0
3	A	14	0	0	3	0
3	B	14	0	0	0	0
3	C	14	0	0	1	0
3	D	14	0	0	1	0
3	F	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	25774	0	26225	2231	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 43.

All (2231) 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:D:159:ILE:CG1	1:D:159:ILE:CD1	1.75	1.60
1:D:39:ILE:CG1	1:D:39:ILE:CD1	1.78	1.55
1:B:430:ILE:CD1	1:B:430:ILE:CG1	1.81	1.54
1:B:133:ILE:CG1	1:B:133:ILE:CD1	1.81	1.53
1:G:472:ILE:HA	1:G:475:ARG:NH1	1.34	1.43
1:E:159:ILE:CG1	1:E:160:GLU:H	1.31	1.33
1:B:440:ILE:CD1	1:B:440:ILE:CB	2.10	1.27
1:B:172:ILE:HD11	1:B:175:CYS:SG	1.76	1.25
1:D:43:THR:O	1:D:44:THR:HG22	1.35	1.24
1:G:472:ILE:HA	1:G:475:ARG:CZ	1.67	1.23
1:A:462:TYR:O	1:A:465:ILE:HD13	1.34	1.22
1:C:59:LEU:HD23	1:C:59:LEU:O	1.39	1.22
1:F:151:TYR:O	1:F:154:VAL:HG22	1.36	1.22
1:F:223:THR:O	1:F:227:LEU:HD23	1.36	1.20
1:G:91:ARG:HH12	1:G:94:VAL:CG1	1.53	1.19
1:F:151:TYR:CE2	1:F:154:VAL:HG21	1.77	1.19
1:C:229:TYR:CD2	1:F:430:ILE:HD11	1.77	1.17
1:G:7:HIS:CD2	1:G:112:PRO:HA	1.80	1.16
1:D:413:LEU:HD11	1:D:415:THR:OG1	1.45	1.16
1:G:339:ARG:CB	1:G:339:ARG:HH11	1.57	1.16
1:C:397:ALA:O	1:C:401:THR:HG23	1.45	1.13
1:C:370:GLY:HA2	2:C:501:U2F:O4	1.45	1.13
1:C:137:THR:OG1	1:C:208:PHE:CD2	1.98	1.12
1:A:58:THR:HA	1:A:61:ASN:ND2	1.65	1.11
1:G:430:ILE:O	1:G:434:THR:HG22	1.50	1.11
1:G:91:ARG:HA	1:G:91:ARG:NH1	1.64	1.11
1:D:372:ASN:HB2	2:D:501:U2F:O1A	1.47	1.10
1:G:89:GLN:HA	1:G:92:LEU:HD21	1.16	1.10
1:G:7:HIS:HD2	1:G:112:PRO:HA	1.11	1.10
1:G:339:ARG:NH1	1:G:339:ARG:HB2	1.64	1.09
1:E:159:ILE:HG13	1:E:160:GLU:N	1.68	1.09
1:E:271:VAL:HG22	1:E:361:SER:O	1.52	1.09
1:G:20:ILE:HG13	1:G:21:PRO:HD3	1.33	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:HA	1:B:295:GLU:CD	1.73	1.09
1:G:81:ASN:O	1:G:84:THR:HG22	1.53	1.09
1:E:159:ILE:CG1	1:E:160:GLU:N	2.11	1.08
1:G:99:PRO:HA	1:G:102:HIS:CD2	1.89	1.08
1:A:44:THR:HG22	1:A:50:GLU:OE1	1.55	1.07
1:C:371:TRP:N	2:C:501:U2F:O4	1.87	1.07
1:A:292:TRP:O	1:A:296:LEU:HD12	1.52	1.06
1:C:370:GLY:CA	2:C:501:U2F:O4	2.03	1.06
1:F:162:GLU:HB2	1:F:165:GLU:OE1	1.56	1.06
1:G:97:ALA:HA	1:G:100:LYS:HE2	1.31	1.06
1:G:124:ILE:CG2	1:G:127:ILE:HD12	1.84	1.06
1:D:396:ASN:O	1:D:400:LEU:HD22	1.55	1.06
1:G:336:PHE:HA	1:G:339:ARG:HH12	1.16	1.05
1:G:472:ILE:HG23	1:G:475:ARG:HH22	0.91	1.05
1:G:137:THR:OG1	1:G:211:ILE:HD12	1.55	1.05
1:G:91:ARG:HH12	1:G:94:VAL:HG13	1.17	1.05
1:E:156:ASP:O	1:E:159:ILE:HD13	1.54	1.05
1:F:290:LEU:CD2	1:F:294:LEU:HD11	1.86	1.05
1:C:14:PRO:CD	1:C:42:ILE:HD11	1.87	1.05
1:G:339:ARG:HH11	1:G:339:ARG:HB2	0.88	1.04
1:G:472:ILE:CA	1:G:475:ARG:NH1	2.19	1.04
1:D:176:LYS:HD2	1:D:403:GLU:OE2	1.56	1.04
1:F:286:GLN:HE22	1:F:419:VAL:CG2	1.71	1.04
1:B:440:ILE:CD1	1:B:440:ILE:HG12	1.53	1.04
1:G:9:ALA:HB3	1:G:115:LEU:CD1	1.88	1.03
1:G:336:PHE:CA	1:G:339:ARG:HH12	1.71	1.03
1:E:159:ILE:HG13	1:E:160:GLU:H	0.89	1.03
1:G:127:ILE:HD13	1:G:128:ALA:N	1.72	1.03
1:B:440:ILE:CG1	1:B:440:ILE:HD12	1.54	1.02
1:E:151:TYR:CZ	1:E:154:VAL:HG21	1.94	1.02
1:E:373:SER:OG	2:E:501:U2F:H5'2	1.59	1.02
1:A:50:GLU:OE2	1:A:51:THR:HG23	1.59	1.02
1:E:147:ALA:HA	1:E:150:ILE:HD11	1.42	1.02
1:D:55:LYS:O	1:D:56:LYS:HG2	1.59	1.02
1:B:440:ILE:CG1	1:B:440:ILE:HD11	1.54	1.01
1:F:151:TYR:CD2	1:F:154:VAL:HG21	1.95	1.01
1:B:109:THR:OG1	1:G:256:ASN:HA	1.60	1.01
1:B:440:ILE:CD1	1:B:440:ILE:HG13	1.53	1.01
1:C:147:ALA:HA	1:C:150:ILE:HD11	1.41	1.01
1:G:328:MET:HA	1:G:328:MET:HE3	1.43	1.00
1:A:106:ALA:HA	1:A:111:ARG:HH22	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ILE:CG1	1:B:440:ILE:HD13	1.54	1.00
1:G:141:THR:HG22	1:G:371:TRP:HB2	1.42	1.00
1:B:327:ASP:O	1:B:328:MET:SD	2.20	1.00
1:G:472:ILE:HG23	1:G:475:ARG:NH2	1.76	1.00
1:C:37:ILE:CD1	1:C:66:ILE:HA	1.90	1.00
1:G:97:ALA:HA	1:G:100:LYS:CE	1.91	0.99
1:C:42:ILE:HA	1:C:71:VAL:HG13	1.43	0.99
1:A:172:ILE:HD11	1:A:175:CYS:C	1.81	0.99
1:G:290:LEU:O	1:G:294:LEU:HD13	1.60	0.99
1:D:396:ASN:O	1:D:400:LEU:CD2	2.10	0.99
1:E:371:TRP:O	1:E:375:VAL:HG13	1.63	0.98
1:A:172:ILE:HD11	1:A:175:CYS:O	1.62	0.98
1:G:91:ARG:HA	1:G:91:ARG:CZ	1.93	0.98
1:F:290:LEU:HD23	1:F:294:LEU:HD11	1.44	0.98
1:G:89:GLN:O	1:G:92:LEU:HD22	1.63	0.97
1:B:33:HIS:ND1	1:B:465:ILE:HG21	1.80	0.97
1:E:122:THR:O	1:E:125:LEU:HG	1.64	0.97
1:G:137:THR:OG1	1:G:211:ILE:CD1	2.12	0.97
1:B:172:ILE:CD1	1:B:175:CYS:SG	2.52	0.97
1:B:392:GLU:OE2	2:B:501:U2F:O4	1.83	0.97
1:G:124:ILE:O	1:G:127:ILE:HG23	1.63	0.97
1:E:284:THR:O	1:E:288:THR:HG23	1.65	0.96
1:E:351:ALA:O	2:E:501:U2F:O7'	1.83	0.96
1:E:372:ASN:HB2	2:E:501:U2F:O1A	1.65	0.96
1:F:286:GLN:HE22	1:F:419:VAL:HG23	1.26	0.96
1:G:124:ILE:HG22	1:G:127:ILE:HD12	1.47	0.96
1:E:244:ILE:CD1	1:E:465:ILE:HG12	1.96	0.96
1:G:141:THR:HG22	1:G:371:TRP:CB	1.96	0.96
1:G:26:GLY:HA2	1:G:29:LEU:HD21	1.45	0.95
1:B:292:TRP:HA	1:B:295:GLU:OE1	1.66	0.95
1:C:59:LEU:HD22	1:C:61:ASN:HD21	1.30	0.94
1:A:106:ALA:N	1:A:111:ARG:HH12	1.65	0.94
1:C:122:THR:O	1:C:123:GLN:O	1.84	0.94
1:G:472:ILE:CG2	1:G:475:ARG:HH22	1.79	0.94
1:D:53:PHE:O	1:D:57:THR:HG22	1.68	0.94
1:C:121:CYS:O	1:C:124:ILE:HG12	1.68	0.94
1:C:14:PRO:HD3	1:C:42:ILE:HD11	1.48	0.94
1:C:59:LEU:O	1:C:59:LEU:CD2	2.16	0.94
1:A:88:THR:O	1:A:92:LEU:HD12	1.66	0.94
1:A:172:ILE:O	1:A:172:ILE:HD13	1.68	0.94
1:D:43:THR:O	1:D:44:THR:CG2	2.15	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:HIS:CE1	1:B:465:ILE:HG21	2.03	0.93
1:C:115:LEU:HD13	1:C:133:ILE:HG21	1.50	0.93
1:D:401:THR:OG1	1:D:409:ARG:NH1	2.01	0.93
1:F:424:ILE:C	1:F:424:ILE:HD13	1.89	0.93
1:F:475:ARG:HD2	1:F:475:ARG:O	1.66	0.93
1:B:401:THR:OG1	1:B:409:ARG:NH1	2.01	0.93
2:C:501:U2F:H3'	2:C:501:U2F:PA	2.09	0.93
1:E:61:ASN:ND2	1:E:66:ILE:H	1.67	0.93
1:F:298:GLN:OE1	1:F:429:ARG:NH2	2.02	0.93
1:A:462:TYR:O	1:A:465:ILE:CD1	2.17	0.93
1:C:137:THR:OG1	1:C:208:PHE:HD2	1.50	0.93
1:F:430:ILE:HA	1:F:434:THR:HG23	1.50	0.92
1:C:350:TRP:CZ2	2:C:501:U2F:O7'	2.22	0.92
1:A:62:GLU:OE1	1:A:66:ILE:HD11	1.67	0.92
1:A:72:PRO:HB2	1:A:100:LYS:HD3	1.52	0.92
1:F:88:THR:O	1:F:92:LEU:HD22	1.69	0.92
1:G:99:PRO:HA	1:G:102:HIS:HD2	1.34	0.92
1:B:440:ILE:CD1	1:B:440:ILE:CG1	0.92	0.92
1:E:75:ASP:O	1:E:78:HIS:CE1	2.23	0.92
1:C:88:THR:O	1:C:92:LEU:HD12	1.70	0.91
1:C:122:THR:C	1:C:123:GLN:O	2.02	0.91
1:F:220:GLU:O	1:F:224:ILE:HG22	1.70	0.91
1:C:57:THR:OG1	1:C:60:THR:HA	1.71	0.91
1:C:19:LEU:O	1:C:22:VAL:HG12	1.70	0.91
1:A:172:ILE:O	1:A:172:ILE:CD1	2.19	0.91
1:D:173:PRO:HB2	1:D:233:LEU:HD22	1.53	0.91
1:A:108:MET:HB2	1:A:111:ARG:NH1	1.86	0.91
1:G:336:PHE:HA	1:G:339:ARG:NH1	1.85	0.91
1:A:108:MET:HB2	1:A:111:ARG:HH11	1.35	0.90
1:A:457:ASP:O	1:A:462:TYR:CD2	2.23	0.90
1:B:88:THR:O	1:B:92:LEU:HD12	1.70	0.90
1:G:89:GLN:HA	1:G:92:LEU:CD2	2.01	0.90
1:G:197:GLU:OE1	1:G:197:GLU:HA	1.67	0.90
1:B:213:ILE:CG2	1:B:215:THR:HG22	2.02	0.90
1:A:430:ILE:HA	1:A:434:THR:HG23	1.54	0.90
1:C:370:GLY:HA2	2:C:501:U2F:HE	1.36	0.89
1:G:89:GLN:O	1:G:92:LEU:CD2	2.20	0.89
1:G:91:ARG:HH12	1:G:94:VAL:HG11	1.34	0.89
1:B:101:ILE:O	1:B:105:ILE:HD12	1.72	0.89
1:E:176:LYS:HE2	1:E:403:GLU:OE2	1.72	0.89
1:G:91:ARG:NH1	1:G:94:VAL:CG1	2.36	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:244:ILE:HD11	1:E:465:ILE:CG1	2.02	0.89
1:D:429:ARG:HB3	1:D:433:GLN:HE22	1.38	0.89
1:A:58:THR:HA	1:A:61:ASN:HD22	1.36	0.88
1:A:426:GLY:O	1:A:430:ILE:HD13	1.73	0.88
1:A:472:ILE:HD13	1:A:473:ARG:N	1.89	0.88
2:C:501:U2F:H4'	2:C:501:U2F:PB	2.13	0.88
1:C:14:PRO:N	1:C:42:ILE:HD11	1.87	0.88
1:E:469:VAL:HA	1:E:472:ILE:HD12	1.55	0.88
1:E:430:ILE:HA	1:E:434:THR:HG23	1.54	0.88
1:E:364:GLY:HA3	1:E:432:MET:HE1	1.56	0.87
1:C:368:HIS:NE2	2:C:501:U2F:O1A	2.08	0.87
1:F:290:LEU:HD23	1:F:294:LEU:CD1	2.04	0.87
1:G:90:LEU:HD13	1:G:91:ARG:N	1.88	0.87
1:A:406:VAL:CG2	1:A:444:ALA:HB2	2.05	0.87
1:B:421:ARG:HA	1:B:424:ILE:HD11	1.57	0.87
1:G:80:ILE:HG13	1:G:84:THR:HG21	1.54	0.87
1:A:92:LEU:HD21	1:B:81:ASN:HD22	1.40	0.87
1:C:159:ILE:HD12	1:C:160:GLU:O	1.74	0.87
1:G:5:GLN:HE22	1:G:36:LYS:HG3	1.40	0.87
1:C:372:ASN:HB2	2:C:501:U2F:H1'	1.55	0.86
1:D:290:LEU:HD22	1:D:303:TRP:CZ2	2.11	0.86
1:E:430:ILE:HA	1:E:434:THR:CG2	2.06	0.86
1:F:76:ILE:O	1:F:76:ILE:HD13	1.75	0.86
1:G:5:GLN:OE1	1:G:35:ILE:HA	1.74	0.86
1:A:430:ILE:HA	1:A:434:THR:CG2	2.06	0.86
1:G:151:TYR:CD1	1:G:154:VAL:HG21	2.11	0.85
1:G:290:LEU:O	1:G:294:LEU:CD1	2.24	0.85
1:G:101:ILE:HD11	1:G:127:ILE:HG21	1.55	0.85
1:B:19:LEU:HD12	1:B:23:LEU:CD2	2.05	0.85
1:G:90:LEU:HD13	1:G:90:LEU:C	1.96	0.85
1:C:350:TRP:HZ2	2:C:501:U2F:O7'	1.58	0.85
1:F:430:ILE:HA	1:F:434:THR:CG2	2.06	0.85
1:G:89:GLN:CA	1:G:92:LEU:HD21	2.03	0.85
1:E:271:VAL:HG23	1:E:362:VAL:HA	1.57	0.85
1:D:429:ARG:CB	1:D:433:GLN:HE22	1.90	0.84
1:E:290:LEU:HD23	1:E:294:LEU:HD11	1.59	0.84
1:F:293:GLY:HA3	1:F:424:ILE:HD12	1.58	0.84
1:G:124:ILE:HG23	1:G:127:ILE:HD12	1.56	0.84
1:A:146:LEU:O	1:A:150:ILE:HD12	1.74	0.84
1:E:185:ASP:HA	1:E:188:LEU:HD23	1.59	0.84
1:A:44:THR:CG2	1:A:50:GLU:OE1	2.26	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:33:HIS:ND1	1:F:465:ILE:HG21	1.92	0.84
1:D:185:ASP:HA	1:D:188:LEU:HD23	1.60	0.84
1:E:159:ILE:CG2	1:E:190:ARG:HH22	1.89	0.84
1:G:197:GLU:O	1:G:200:LYS:HG3	1.78	0.84
1:C:37:ILE:HD11	1:C:66:ILE:HB	1.60	0.84
1:F:441:LYS:O	1:F:445:LYS:NZ	2.09	0.84
1:C:229:TYR:CE2	1:F:430:ILE:HD11	2.12	0.83
1:F:151:TYR:HD2	1:F:155:PHE:CE2	1.96	0.83
1:F:223:THR:O	1:F:227:LEU:CD2	2.25	0.83
1:G:7:HIS:CD2	1:G:112:PRO:CA	2.60	0.83
1:G:33:HIS:ND1	1:G:465:ILE:HG21	1.91	0.83
1:G:151:TYR:CE1	1:G:154:VAL:HG21	2.13	0.83
1:F:326:ARG:HG3	1:F:330:GLU:OE2	1.78	0.83
1:B:185:ASP:HA	1:B:188:LEU:HD23	1.60	0.83
1:G:377:SER:O	1:G:382:VAL:HG22	1.78	0.83
1:A:106:ALA:HA	1:A:111:ARG:NH2	1.93	0.83
1:G:185:ASP:HA	1:G:188:LEU:HD23	1.61	0.83
1:D:413:LEU:HD22	1:D:414:PRO:HD2	1.61	0.83
1:F:154:VAL:HG23	1:F:155:PHE:N	1.92	0.83
1:G:76:ILE:HG13	1:G:76:ILE:O	1.78	0.83
1:C:109:THR:HG23	1:C:110:HIS:ND1	1.94	0.82
1:F:192:ASP:OD1	1:F:194:GLN:OE1	1.96	0.82
1:E:180:PRO:O	1:E:183:VAL:HG12	1.78	0.82
1:E:183:VAL:CG2	1:E:187:LEU:HB2	2.08	0.82
1:G:170:LEU:CD2	1:G:178:LEU:HB3	2.09	0.82
1:G:474:SER:O	1:G:475:ARG:HD3	1.79	0.82
1:F:286:GLN:NE2	1:F:419:VAL:CG2	2.41	0.82
1:F:286:GLN:NE2	1:F:419:VAL:HG23	1.93	0.82
1:A:231:GLU:O	1:A:235:LEU:HD12	1.79	0.82
1:A:341:LYS:HD2	1:A:342:ASP:OD1	1.80	0.82
1:E:413:LEU:HD12	1:E:414:PRO:HD2	1.61	0.82
1:F:188:LEU:HD23	1:F:188:LEU:N	1.94	0.82
1:G:137:THR:HG1	1:G:211:ILE:HD12	1.45	0.82
1:A:210:GLY:C	1:A:211:ILE:HD12	2.01	0.82
1:A:377:SER:O	1:A:382:VAL:HG22	1.79	0.81
1:G:170:LEU:CD2	1:G:178:LEU:CB	2.58	0.81
1:G:116:ILE:HD11	1:G:138:TYR:HB2	1.61	0.81
1:A:63:GLU:O	1:A:63:GLU:HG2	1.80	0.81
1:E:424:ILE:O	1:E:428:VAL:HG12	1.80	0.81
1:C:377:SER:OG	1:C:382:VAL:HG23	1.80	0.81
1:B:377:SER:O	1:B:382:VAL:HG22	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HG	1:A:472:ILE:HD11	1.62	0.81
1:B:109:THR:HG23	1:G:255:LEU:C	2.01	0.81
1:A:131:PHE:HB2	1:A:133:ILE:HD11	1.62	0.81
1:A:377:SER:OG	1:A:382:VAL:HG23	1.81	0.81
1:E:115:LEU:HD23	1:E:133:ILE:HG21	1.60	0.81
1:E:86:ILE:O	1:E:90:LEU:HD12	1.81	0.81
1:E:146:LEU:O	1:E:150:ILE:HD13	1.81	0.81
1:G:125:LEU:HG	1:G:126:PRO:HD3	1.63	0.81
1:B:291:ALA:O	1:B:295:GLU:OE1	1.99	0.80
1:B:112:PRO:O	1:B:133:ILE:HG12	1.80	0.80
1:E:19:LEU:HD13	1:E:23:LEU:HD13	1.63	0.80
2:E:501:U2F:H3'	2:E:501:U2F:O6'	1.82	0.80
1:F:25:LEU:O	1:F:29:LEU:HD12	1.80	0.80
1:B:337:LEU:O	1:B:341:LYS:HG3	1.81	0.80
1:D:263:LEU:HB3	1:D:359:HIS:ND1	1.97	0.80
1:F:263:LEU:HB3	1:F:359:HIS:HD1	1.45	0.80
1:G:98:LEU:HD23	1:G:98:LEU:C	2.01	0.80
1:C:429:ARG:HH12	1:D:260:ILE:CG2	1.94	0.80
1:E:284:THR:HG23	1:E:310:ASP:OD2	1.82	0.80
1:G:91:ARG:NH1	1:G:94:VAL:HG13	1.95	0.80
1:G:106:ALA:HA	1:G:108:MET:SD	2.22	0.80
1:C:59:LEU:HD21	1:C:67:GLU:HG3	1.63	0.80
1:F:173:PRO:HB3	1:F:232:LYS:HD2	1.63	0.80
1:C:377:SER:O	1:C:382:VAL:HG22	1.81	0.80
2:C:501:U2F:H4'	2:C:501:U2F:O1B	1.82	0.80
1:B:393:GLN:HE21	2:B:501:U2F:C6	1.94	0.80
1:D:231:GLU:O	1:D:235:LEU:HD12	1.81	0.80
1:D:263:LEU:HB3	1:D:359:HIS:HD1	1.45	0.80
1:E:244:ILE:CD1	1:E:465:ILE:CG1	2.58	0.80
1:B:239:VAL:HG23	1:B:240:PRO:HD2	1.63	0.80
1:B:251:VAL:HG12	1:B:354:VAL:HG22	1.63	0.80
2:C:501:U2F:H5'1	2:C:501:U2F:H9'	1.62	0.80
1:E:263:LEU:HB3	1:E:359:HIS:ND1	1.96	0.80
1:G:424:ILE:O	1:G:428:VAL:HG12	1.82	0.80
1:C:60:THR:C	1:C:61:ASN:HD22	1.85	0.79
1:F:263:LEU:HB3	1:F:359:HIS:ND1	1.96	0.79
1:C:328:MET:HA	1:C:328:MET:HE3	1.62	0.79
2:C:501:U2F:C3'	2:C:501:U2F:O3A	2.30	0.79
1:A:184:VAL:HG13	1:A:395:MET:HE3	1.64	0.79
1:C:37:ILE:HD13	1:C:66:ILE:HA	1.63	0.79
1:C:109:THR:HG23	1:C:110:HIS:CE1	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:GLU:HB2	1:F:165:GLU:CD	2.02	0.79
1:E:295:GLU:OE1	1:E:339:ARG:NH1	2.15	0.79
1:B:151:TYR:HD2	1:B:155:PHE:CE2	2.01	0.79
1:F:95:ARG:NH2	1:F:123:GLN:HE22	1.80	0.79
1:G:8:VAL:HG22	1:G:37:ILE:HG12	1.65	0.79
1:G:183:VAL:O	1:G:394:LYS:HD2	1.82	0.79
1:A:14:PRO:HG3	1:A:93:LEU:HD22	1.65	0.79
1:C:290:LEU:O	1:C:294:LEU:HD23	1.83	0.79
1:D:151:TYR:HD2	1:D:155:PHE:CE2	2.01	0.79
1:B:110:HIS:NE2	1:G:255:LEU:HG	1.98	0.79
1:D:337:LEU:H	1:D:337:LEU:HD22	1.47	0.79
1:G:20:ILE:CG1	1:G:21:PRO:HD3	2.13	0.79
1:E:125:LEU:CD1	1:E:126:PRO:HD3	2.13	0.78
1:E:290:LEU:CD2	1:E:294:LEU:HD11	2.12	0.78
1:F:424:ILE:O	1:F:428:VAL:HG12	1.82	0.78
1:C:397:ALA:O	1:C:401:THR:CG2	2.29	0.78
1:G:151:TYR:O	1:G:154:VAL:HG23	1.82	0.78
1:A:172:ILE:O	1:A:172:ILE:CG1	2.30	0.78
1:G:170:LEU:HD23	1:G:178:LEU:HB3	1.65	0.78
1:B:19:LEU:HD12	1:B:23:LEU:HD21	1.66	0.78
1:G:170:LEU:HD11	1:G:177:ALA:HA	1.63	0.78
1:E:151:TYR:HD2	1:E:155:PHE:CE2	2.01	0.78
1:A:92:LEU:CD2	1:B:81:ASN:HD22	1.97	0.77
1:F:219:LEU:HD12	1:F:220:GLU:HG3	1.66	0.77
1:F:426:GLY:O	1:F:430:ILE:CD1	2.32	0.77
1:G:234:ARG:HH11	1:G:238:LYS:NZ	1.81	0.77
1:A:19:LEU:O	1:A:23:LEU:HD13	1.83	0.77
1:F:248:ARG:CD	1:F:379:THR:HG21	2.14	0.77
1:G:272:LEU:HD23	1:G:428:VAL:HG23	1.65	0.77
1:F:244:ILE:HA	1:F:461:SER:OG	1.83	0.77
1:C:185:ASP:HA	1:C:188:LEU:HD13	1.64	0.77
1:E:74:VAL:HG13	1:E:76:ILE:CD1	2.14	0.77
1:F:441:LYS:HG3	1:F:445:LYS:HZ1	1.48	0.77
1:D:467:GLU:O	1:D:470:LYS:HG3	1.85	0.77
1:G:91:ARG:NH1	1:G:94:VAL:HG11	2.00	0.77
1:G:471:ASP:O	1:G:475:ARG:HD2	1.83	0.77
1:G:290:LEU:HD23	1:G:294:LEU:HD11	1.65	0.77
1:C:151:TYR:HD2	1:C:155:PHE:CE2	2.01	0.77
1:F:260:ILE:CG2	1:G:429:ARG:HH12	1.97	0.76
1:C:59:LEU:HD21	1:C:67:GLU:CG	2.15	0.76
1:C:71:VAL:HG23	1:C:100:LYS:HD2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:TRP:O	1:D:264:ASP:N	2.17	0.76
1:F:131:PHE:HB2	1:F:133:ILE:CD1	2.16	0.76
1:D:429:ARG:O	1:D:433:GLN:OE1	2.04	0.76
1:G:10:ILE:HD13	1:G:25:LEU:HD22	1.65	0.76
1:G:25:LEU:HD23	1:G:29:LEU:HD22	1.67	0.76
1:D:396:ASN:H	1:D:396:ASN:HD22	1.33	0.76
1:F:86:ILE:HD12	1:F:86:ILE:H	1.49	0.76
1:B:352:ASN:HB3	1:B:355:GLU:OE1	1.85	0.76
1:C:330:GLU:HG3	1:C:331:TYR:CD1	2.20	0.76
2:C:501:U2F:H3'	2:C:501:U2F:O3A	1.85	0.76
1:E:122:THR:O	1:E:125:LEU:CG	2.34	0.76
1:B:371:TRP:O	1:B:375:VAL:HG22	1.86	0.76
1:E:147:ALA:HA	1:E:150:ILE:CD1	2.14	0.75
1:D:429:ARG:HA	1:D:433:GLN:OE1	1.86	0.75
1:F:424:ILE:C	1:F:424:ILE:CD1	2.53	0.75
1:C:332:LEU:HD11	1:C:336:PHE:HB3	1.68	0.75
1:G:25:LEU:O	1:G:29:LEU:CD2	2.35	0.75
1:G:88:THR:O	1:G:92:LEU:HD13	1.87	0.75
1:G:170:LEU:HD12	1:G:171:LYS:N	2.02	0.75
2:D:501:U2F:H5'2	2:D:501:U2F:H9'	1.68	0.75
1:G:8:VAL:H	1:G:37:ILE:CG1	1.98	0.75
1:G:472:ILE:HA	1:G:475:ARG:HH12	1.46	0.75
1:C:461:SER:O	1:C:465:ILE:HD12	1.87	0.75
1:A:101:ILE:HD13	1:A:102:HIS:N	2.02	0.75
1:G:328:MET:HE3	1:G:331:TYR:CE2	2.21	0.75
1:B:292:TRP:CA	1:B:295:GLU:OE1	2.34	0.74
1:B:295:GLU:HB2	1:B:339:ARG:HH12	1.52	0.74
1:C:370:GLY:C	2:C:501:U2F:O4	2.25	0.74
1:E:119:ILE:CG2	1:E:140:PRO:HD3	2.16	0.74
1:C:297:SER:HB3	1:C:428:VAL:HG21	1.69	0.74
1:F:426:GLY:O	1:F:430:ILE:HD13	1.88	0.74
1:B:259:VAL:HG12	1:B:345:LEU:HD23	1.67	0.74
1:G:153:GLN:HE21	1:G:203:LYS:HE3	1.52	0.74
1:G:170:LEU:HD11	1:G:178:LEU:H	1.52	0.74
1:A:426:GLY:O	1:A:430:ILE:CD1	2.35	0.74
1:F:151:TYR:CD2	1:F:154:VAL:CG2	2.70	0.74
1:G:97:ALA:CA	1:G:100:LYS:HE2	2.13	0.74
1:A:81:ASN:ND2	1:B:192:ASP:OD1	2.20	0.74
1:A:92:LEU:HD21	1:B:81:ASN:ND2	2.02	0.74
2:A:501:U2F:H6C1	3:A:502:T83:OAC	1.88	0.74
2:C:501:U2F:O3A	2:C:501:U2F:HC	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:LEU:HD23	1:E:294:LEU:CD1	2.18	0.74
1:F:374:THR:CG2	1:F:400:LEU:HD21	2.18	0.74
1:A:228:ARG:HA	1:A:234:ARG:HH21	1.53	0.73
1:C:435:LYS:NZ	1:D:382:VAL:HG22	2.03	0.73
1:F:16:MET:HE1	1:F:53:PHE:CD2	2.23	0.73
1:F:293:GLY:CA	1:F:424:ILE:HD12	2.17	0.73
1:D:367:THR:HG23	1:D:369:CYS:H	1.53	0.73
1:E:115:LEU:HD23	1:E:133:ILE:CG2	2.18	0.73
1:E:438:LYS:N	1:E:438:LYS:HD2	2.03	0.73
1:C:109:THR:CG2	1:C:110:HIS:CE1	2.70	0.73
1:E:151:TYR:CE2	1:E:154:VAL:HG21	2.23	0.73
1:G:179:ARG:HD2	1:G:180:PRO:HD2	1.69	0.73
1:E:159:ILE:HG21	1:E:190:ARG:HH12	1.53	0.73
1:E:203:LYS:O	1:E:206:THR:HG22	1.87	0.73
1:A:50:GLU:HG2	1:A:51:THR:N	2.01	0.73
1:A:462:TYR:C	1:A:465:ILE:HD13	2.08	0.73
1:B:374:THR:CG2	1:B:400:LEU:HD21	2.19	0.73
1:F:441:LYS:CG	1:F:445:LYS:HZ1	2.01	0.73
1:G:367:THR:HG23	1:G:369:CYS:H	1.51	0.73
1:C:44:THR:HG21	1:C:47:SER:HB3	1.71	0.73
1:F:469:VAL:HA	1:F:472:ILE:CD1	2.19	0.73
1:G:88:THR:HG23	1:G:194:GLN:HB3	1.71	0.73
1:D:429:ARG:HB3	1:D:433:GLN:NE2	2.04	0.73
1:A:262:TRP:CG	1:A:345:LEU:HD13	2.23	0.72
1:C:57:THR:OG1	1:C:60:THR:CA	2.37	0.72
1:D:392:GLU:HG2	1:D:396:ASN:ND2	2.05	0.72
1:F:251:VAL:HG23	1:F:354:VAL:HG12	1.69	0.72
1:G:339:ARG:HH11	1:G:339:ARG:CG	2.01	0.72
1:C:147:ALA:HA	1:C:150:ILE:CD1	2.16	0.72
1:C:306:ARG:HA	1:C:349:MET:HE1	1.70	0.72
1:G:74:VAL:HG13	1:G:100:LYS:HE3	1.71	0.72
1:G:170:LEU:CD1	1:G:171:LYS:N	2.52	0.72
1:B:412:VAL:HG11	1:B:417:LYS:HE3	1.70	0.72
1:B:400:LEU:HA	1:B:404:LEU:HD12	1.71	0.72
1:C:59:LEU:HG	1:C:68:ILE:O	1.88	0.72
1:E:61:ASN:ND2	1:E:66:ILE:N	2.37	0.72
1:G:9:ALA:HB3	1:G:115:LEU:HD11	1.68	0.72
1:G:197:GLU:OE1	1:G:197:GLU:CA	2.38	0.72
1:B:213:ILE:HG21	1:B:215:THR:HG22	1.70	0.72
1:E:119:ILE:HG13	1:E:120:PHE:CD1	2.23	0.72
1:A:203:LYS:O	1:A:206:THR:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:ASN:HB3	1:E:355:GLU:OE1	1.90	0.72
1:G:170:LEU:HD21	1:G:178:LEU:HB2	1.70	0.72
1:E:163:TYR:CZ	1:E:190:ARG:NH2	2.57	0.72
1:D:392:GLU:HG2	1:D:396:ASN:HD21	1.54	0.71
1:E:263:LEU:HB3	1:E:359:HIS:CE1	2.24	0.71
1:B:172:ILE:O	1:B:172:ILE:HD13	1.90	0.71
1:A:20:ILE:HG12	1:A:21:PRO:HD3	1.72	0.71
1:D:413:LEU:HD13	1:D:416:LYS:H	1.54	0.71
1:E:125:LEU:HD12	1:E:126:PRO:HD3	1.72	0.71
1:F:425:GLN:HE21	1:F:429:ARG:HE	1.36	0.71
1:G:463:ASN:O	1:G:466:CYS:SG	2.47	0.71
1:C:373:SER:OG	2:C:501:U2F:O2'	2.03	0.71
1:E:216:TRP:CH2	1:E:219:LEU:HD23	2.25	0.71
1:B:239:VAL:CG2	1:B:240:PRO:HD2	2.21	0.71
1:F:263:LEU:HB3	1:F:359:HIS:CE1	2.25	0.71
1:G:469:VAL:HA	1:G:472:ILE:HG12	1.72	0.71
1:B:213:ILE:HG22	1:B:215:THR:H	1.55	0.71
1:G:108:MET:O	1:G:108:MET:HG2	1.90	0.71
1:D:203:LYS:O	1:D:206:THR:HG22	1.89	0.71
1:C:176:LYS:HG2	1:C:177:ALA:H	1.53	0.70
1:A:420:LYS:O	1:A:424:ILE:HD12	1.91	0.70
1:F:203:LYS:O	1:F:206:THR:HG22	1.91	0.70
1:F:151:TYR:O	1:F:154:VAL:CG2	2.29	0.70
1:G:9:ALA:HB3	1:G:115:LEU:HD13	1.72	0.70
1:G:251:VAL:HG12	1:G:252:GLU:H	1.56	0.70
1:B:338:THR:HA	1:B:341:LYS:HD2	1.73	0.70
1:F:406:VAL:HG11	1:F:447:LEU:HD12	1.73	0.70
1:B:440:ILE:HD12	1:B:440:ILE:N	2.07	0.70
1:G:105:ILE:HD12	1:G:108:MET:HB3	1.73	0.70
1:B:421:ARG:HA	1:B:424:ILE:CD1	2.22	0.70
1:C:42:ILE:O	1:C:42:ILE:HD13	1.92	0.70
1:C:178:LEU:CD1	1:C:183:VAL:HG12	2.20	0.70
1:D:98:LEU:HA	1:D:101:ILE:CD1	2.21	0.70
1:G:90:LEU:CD1	1:G:91:ARG:HH11	2.05	0.70
1:E:44:THR:HG21	1:E:47:SER:OG	1.91	0.70
1:G:352:ASN:HB3	1:G:355:GLU:OE1	1.92	0.70
1:E:18:HIS:O	1:E:22:VAL:HG13	1.92	0.70
1:F:151:TYR:CE2	1:F:154:VAL:CG2	2.67	0.70
1:B:137:THR:HG21	1:B:205:TYR:CD1	2.27	0.69
1:C:12:SER:O	1:C:42:ILE:HD12	1.91	0.69
1:C:37:ILE:HD11	1:C:66:ILE:HA	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:TRP:CH2	1:F:219:LEU:HD23	2.27	0.69
1:F:364:GLY:HA3	1:F:432:MET:CE	2.22	0.69
1:G:19:LEU:O	1:G:23:LEU:HD23	1.91	0.69
1:C:262:TRP:CZ3	1:C:266:GLN:HG3	2.27	0.69
1:G:203:LYS:O	1:G:206:THR:HG22	1.91	0.69
1:G:244:ILE:H	1:G:244:ILE:HD13	1.57	0.69
1:C:59:LEU:CD2	1:C:67:GLU:HG3	2.21	0.69
1:D:18:HIS:O	1:D:22:VAL:CG2	2.40	0.69
1:G:19:LEU:HD13	1:G:23:LEU:HD23	1.74	0.69
1:G:166:LEU:HD12	1:G:168:GLU:HB2	1.74	0.69
1:C:203:LYS:O	1:C:206:THR:HG22	1.91	0.69
1:E:421:ARG:HA	1:E:424:ILE:HD12	1.73	0.69
1:F:293:GLY:HA3	1:F:424:ILE:CD1	2.22	0.69
1:B:454:ALA:HB1	1:B:461:SER:OG	1.92	0.69
1:B:293:GLY:HA3	1:B:424:ILE:HG13	1.74	0.69
1:E:244:ILE:HD11	1:E:465:ILE:HG13	1.75	0.69
1:F:50:GLU:O	1:F:54:LEU:HD23	1.92	0.69
1:F:60:THR:OG1	1:F:61:ASN:N	2.24	0.69
1:F:286:GLN:HE22	1:F:419:VAL:HG22	1.53	0.69
1:F:368:HIS:HB2	1:F:389:LEU:HD23	1.74	0.69
1:B:146:LEU:HD22	1:B:213:ILE:HD11	1.73	0.69
1:D:292:TRP:O	1:D:296:LEU:HD12	1.92	0.69
1:F:474:SER:O	1:F:477:LEU:CD1	2.41	0.69
1:G:305:VAL:CG2	1:G:328:MET:HE2	2.23	0.69
1:A:80:ILE:HG12	1:A:84:THR:HB	1.75	0.69
1:A:172:ILE:O	1:A:172:ILE:HG12	1.93	0.69
1:C:244:ILE:HD13	1:C:244:ILE:H	1.58	0.69
1:D:449:LYS:O	1:D:453:ASN:ND2	2.25	0.69
1:B:101:ILE:O	1:B:105:ILE:CD1	2.40	0.68
1:B:172:ILE:HD13	1:B:172:ILE:C	2.13	0.68
1:E:118:ASP:HB3	1:E:121:CYS:SG	2.33	0.68
1:E:246:PRO:HD2	1:E:455:LEU:CD1	2.24	0.68
1:A:106:ALA:N	1:A:111:ARG:NH1	2.40	0.68
1:D:263:LEU:HB3	1:D:359:HIS:CE1	2.27	0.68
1:B:244:ILE:H	1:B:244:ILE:HD13	1.56	0.68
1:D:184:VAL:HG23	1:D:187:LEU:HD13	1.75	0.68
1:G:29:LEU:HD23	1:G:29:LEU:H	1.59	0.68
1:A:457:ASP:O	1:A:462:TYR:CE2	2.46	0.68
1:C:6:LEU:HD22	1:C:473:ARG:CZ	2.24	0.68
1:E:176:LYS:HE2	1:E:403:GLU:CD	2.14	0.68
1:A:62:GLU:OE1	1:A:66:ILE:CD1	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:VAL:HA	1:A:472:ILE:CG2	2.24	0.68
1:A:473:ARG:O	1:A:477:LEU:HD13	1.94	0.68
1:A:172:ILE:HD12	1:A:176:LYS:O	1.94	0.68
1:F:387:TRP:O	1:F:389:LEU:HD22	1.94	0.68
1:G:8:VAL:HG22	1:G:37:ILE:CD1	2.23	0.68
1:G:8:VAL:H	1:G:37:ILE:HG13	1.57	0.68
1:E:87:PHE:HB3	1:E:194:GLN:HE21	1.57	0.67
1:F:154:VAL:CG2	1:F:155:PHE:N	2.56	0.67
1:G:305:VAL:HG23	1:G:328:MET:HE2	1.74	0.67
1:A:30:ALA:HB1	1:A:65:THR:OG1	1.94	0.67
1:C:12:SER:HB2	1:C:22:VAL:HG11	1.76	0.67
1:C:41:ALA:O	1:C:71:VAL:HG12	1.94	0.67
1:C:213:ILE:HD12	1:C:241:VAL:HG22	1.76	0.67
1:F:239:VAL:HG23	1:F:240:PRO:HD2	1.77	0.67
1:A:33:HIS:CE1	1:A:465:ILE:HG13	2.29	0.67
1:C:150:ILE:H	1:C:150:ILE:HD13	1.60	0.67
1:F:290:LEU:CD2	1:F:294:LEU:CD1	2.64	0.67
1:D:95:ARG:HD3	1:D:123:GLN:NE2	2.10	0.67
1:D:290:LEU:O	1:D:294:LEU:HD12	1.95	0.67
1:D:424:ILE:HA	1:D:427:MET:HE2	1.76	0.67
1:F:290:LEU:HD21	1:F:294:LEU:HD11	1.75	0.67
1:G:294:LEU:HD12	1:G:294:LEU:N	2.10	0.67
1:G:430:ILE:O	1:G:434:THR:CG2	2.36	0.67
1:A:20:ILE:CG1	1:A:21:PRO:HD3	2.24	0.67
1:B:374:THR:HG21	1:B:400:LEU:HD21	1.76	0.67
1:D:212:LEU:HD23	1:D:244:ILE:HD13	1.77	0.67
1:G:18:HIS:O	1:G:22:VAL:CG2	2.43	0.67
1:D:10:ILE:CG2	1:D:22:VAL:HG12	2.25	0.66
1:C:37:ILE:HD11	1:C:66:ILE:CB	2.24	0.66
1:E:50:GLU:O	1:E:54:LEU:HD23	1.95	0.66
1:F:95:ARG:NH2	1:F:123:GLN:NE2	2.44	0.66
1:F:95:ARG:HH21	1:F:123:GLN:NE2	1.93	0.66
1:F:188:LEU:N	1:F:188:LEU:CD2	2.57	0.66
1:A:249:ARG:CZ	1:A:354:VAL:HG23	2.24	0.66
1:D:335:GLY:O	1:D:337:LEU:N	2.29	0.66
1:G:153:GLN:HE21	1:G:203:LYS:CE	2.08	0.66
1:G:179:ARG:CD	1:G:180:PRO:HD2	2.24	0.66
1:G:269:GLU:OE1	1:G:441:LYS:NZ	2.28	0.66
1:E:364:GLY:CA	1:E:432:MET:HE1	2.25	0.66
1:B:436:GLU:O	1:B:440:ILE:HD13	1.95	0.66
1:C:213:ILE:O	1:C:244:ILE:HD13	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:372:ASN:CB	2:D:501:U2F:O1A	2.34	0.66
1:E:6:LEU:HD11	1:E:473:ARG:HD3	1.76	0.66
1:E:327:ASP:OD1	1:E:328:MET:N	2.28	0.66
1:B:285:LYS:NZ	1:B:289:GLU:HG2	2.09	0.66
1:E:249:ARG:NH2	2:E:501:U2F:H3	1.93	0.66
1:B:327:ASP:C	1:B:328:MET:SD	2.74	0.66
1:C:159:ILE:HG13	1:C:166:LEU:HD21	1.78	0.66
1:C:7:HIS:ND1	1:C:112:PRO:HA	2.10	0.66
1:E:290:LEU:O	1:E:294:LEU:HD12	1.95	0.66
1:G:155:PHE:HZ	1:G:172:ILE:HD13	1.61	0.66
1:C:112:PRO:O	1:C:133:ILE:HD12	1.95	0.66
1:E:14:PRO:O	1:E:50:GLU:OE1	2.12	0.66
1:F:75:ASP:O	1:F:76:ILE:HG22	1.96	0.66
1:F:290:LEU:O	1:F:294:LEU:HD12	1.96	0.66
1:D:95:ARG:NE	1:D:123:GLN:NE2	2.43	0.66
1:C:292:TRP:O	1:C:296:LEU:HD22	1.96	0.65
1:E:372:ASN:ND2	2:E:501:U2F:O1A	2.29	0.65
1:F:469:VAL:HA	1:F:472:ILE:HD11	1.77	0.65
1:C:37:ILE:HD13	1:C:37:ILE:O	1.95	0.65
1:E:74:VAL:HG13	1:E:76:ILE:HD11	1.77	0.65
1:G:25:LEU:HD23	1:G:25:LEU:C	2.16	0.65
1:G:101:ILE:CD1	1:G:127:ILE:HG21	2.25	0.65
1:A:193:GLN:O	1:A:196:GLU:HG2	1.95	0.65
1:D:117:VAL:HG13	1:D:121:CYS:HB2	1.78	0.65
1:E:75:ASP:O	1:E:78:HIS:NE2	2.29	0.65
1:F:12:SER:OG	1:F:41:ALA:HA	1.97	0.65
1:G:170:LEU:HD21	1:G:178:LEU:CB	2.25	0.65
1:C:7:HIS:CD2	1:C:36:LYS:HD2	2.32	0.65
1:D:117:VAL:HG11	1:D:121:CYS:O	1.96	0.65
1:E:87:PHE:CB	1:E:194:GLN:HE21	2.08	0.65
1:A:290:LEU:O	1:A:294:LEU:HD12	1.96	0.65
1:B:112:PRO:O	1:B:133:ILE:CG1	2.45	0.65
1:B:290:LEU:O	1:B:294:LEU:HD12	1.96	0.65
1:C:328:MET:HA	1:C:328:MET:CE	2.25	0.65
1:E:255:LEU:HG	1:E:256:ASN:H	1.60	0.65
1:E:271:VAL:CG2	1:E:361:SER:O	2.39	0.65
1:G:455:LEU:O	1:G:456:SER:OG	2.12	0.65
1:F:387:TRP:O	1:F:389:LEU:CD2	2.45	0.65
1:A:377:SER:OG	1:A:382:VAL:CG2	2.45	0.65
2:E:501:U2F:O6'	2:E:501:U2F:C3'	2.45	0.65
1:E:115:LEU:CD2	1:E:133:ILE:HG21	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ALA:H	1:A:111:ARG:HH12	1.44	0.64
1:C:371:TRP:N	2:C:501:U2F:HE	1.95	0.64
1:E:148:LEU:HD12	1:E:198:TYR:OH	1.97	0.64
1:G:11:VAL:HG22	1:G:40:LEU:HB3	1.78	0.64
1:G:125:LEU:HG	1:G:126:PRO:CD	2.27	0.64
1:B:146:LEU:CD2	1:B:213:ILE:HD11	2.27	0.64
1:G:90:LEU:HD11	1:G:120:PHE:HB3	1.78	0.64
1:F:213:ILE:O	1:F:244:ILE:HD13	1.97	0.64
1:G:213:ILE:O	1:G:244:ILE:HD13	1.96	0.64
1:G:366:LEU:HD22	1:G:385:ILE:HB	1.79	0.64
1:C:117:VAL:HG11	1:C:121:CYS:O	1.98	0.64
1:G:51:THR:O	1:G:54:LEU:HG	1.97	0.64
1:G:80:ILE:HG13	1:G:84:THR:CG2	2.25	0.64
1:C:8:VAL:HG22	1:C:114:ALA:HB3	1.79	0.64
1:D:33:HIS:CD2	1:D:465:ILE:HG21	2.33	0.64
1:D:176:LYS:CD	1:D:403:GLU:OE2	2.42	0.64
1:F:374:THR:HG21	1:F:400:LEU:HD21	1.79	0.64
1:C:117:VAL:HG13	1:C:121:CYS:HB2	1.79	0.64
1:E:154:VAL:O	1:E:157:LYS:HG2	1.98	0.64
1:F:244:ILE:CA	1:F:461:SER:OG	2.45	0.64
1:G:25:LEU:O	1:G:29:LEU:HD22	1.97	0.64
1:G:26:GLY:CA	1:G:29:LEU:HD21	2.25	0.64
1:G:471:ASP:O	1:G:475:ARG:CD	2.46	0.64
1:A:14:PRO:CG	1:A:42:ILE:HD11	2.28	0.64
1:C:13:SER:C	1:C:42:ILE:HD11	2.18	0.64
1:E:119:ILE:CG2	1:E:140:PRO:CD	2.75	0.64
1:G:8:VAL:CG2	1:G:37:ILE:HG12	2.28	0.64
1:C:76:ILE:CD1	1:C:93:LEU:HD22	2.28	0.64
1:D:424:ILE:HA	1:D:427:MET:CE	2.27	0.64
1:F:126:PRO:HA	1:F:129:GLU:OE1	1.97	0.64
1:A:33:HIS:CE1	1:A:465:ILE:HD11	2.33	0.64
1:C:377:SER:OG	1:C:382:VAL:CG2	2.45	0.64
1:D:10:ILE:HG22	1:D:22:VAL:HG12	1.80	0.64
1:D:173:PRO:HB2	1:D:233:LEU:CD2	2.25	0.64
1:B:166:LEU:O	1:B:167:LYS:HG2	1.98	0.63
1:E:73:SER:HB2	1:E:93:LEU:HD21	1.79	0.63
1:F:381:GLY:O	1:F:445:LYS:NZ	2.30	0.63
1:G:76:ILE:HD13	1:G:96:GLU:HG3	1.80	0.63
1:D:106:ALA:HA	1:D:111:ARG:HH12	1.61	0.63
1:F:248:ARG:NE	1:F:379:THR:HG21	2.13	0.63
1:G:89:GLN:C	1:G:92:LEU:HD22	2.19	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:141:THR:HG21	1:G:392:GLU:OE2	1.98	0.63
1:G:246:PRO:HB2	1:G:375:VAL:HG13	1.81	0.63
1:A:246:PRO:HB2	1:A:375:VAL:HG13	1.80	0.63
1:C:13:SER:C	1:C:42:ILE:CD1	2.67	0.63
1:D:246:PRO:HB2	1:D:375:VAL:HG13	1.81	0.63
1:G:52:GLU:O	1:G:56:LYS:CG	2.46	0.63
2:C:501:U2F:PA	2:C:501:U2F:C3'	2.85	0.63
1:E:281:THR:HG21	1:E:309:SER:HB3	1.80	0.63
1:G:387:TRP:HH2	1:G:424:ILE:HD11	1.62	0.63
1:E:7:HIS:HB2	1:E:110:HIS:NE2	2.14	0.63
1:E:246:PRO:HD2	1:E:455:LEU:HD11	1.79	0.63
1:E:396:ASN:O	1:E:400:LEU:HD12	1.99	0.63
1:G:170:LEU:HD23	1:G:178:LEU:CB	2.25	0.63
1:G:176:LYS:HG2	1:G:177:ALA:H	1.63	0.63
1:G:455:LEU:O	1:G:456:SER:CB	2.46	0.63
1:E:32:HIS:HB2	1:E:33:HIS:CE1	2.32	0.63
1:F:424:ILE:HD13	1:F:424:ILE:O	1.98	0.63
1:G:20:ILE:HD12	1:G:21:PRO:N	2.14	0.63
1:B:148:LEU:HD22	1:B:178:LEU:HD12	1.80	0.63
1:D:396:ASN:HD22	1:D:396:ASN:N	1.97	0.63
1:G:290:LEU:HD23	1:G:294:LEU:CD1	2.27	0.63
1:C:476:GLU:O	1:C:477:LEU:HG	1.99	0.63
1:F:441:LYS:C	1:F:445:LYS:HZ3	2.01	0.63
1:C:329:SER:HA	1:C:332:LEU:HD22	1.80	0.62
1:A:125:LEU:HD12	1:A:135:LYS:HD2	1.81	0.62
1:E:77:SER:HA	1:E:80:ILE:CD1	2.29	0.62
1:B:159:ILE:H	1:B:159:ILE:HD12	1.64	0.62
1:D:95:ARG:CD	1:D:123:GLN:NE2	2.63	0.62
1:E:12:SER:HB2	1:E:22:VAL:HG21	1.81	0.62
1:G:170:LEU:HD22	1:G:172:ILE:HD11	1.81	0.62
1:A:6:LEU:CG	1:A:472:ILE:HD11	2.29	0.62
1:A:136:TYR:OH	1:A:471:ASP:OD1	2.17	0.62
1:C:37:ILE:CD1	1:C:66:ILE:CA	2.72	0.62
1:F:25:LEU:O	1:F:29:LEU:CD1	2.46	0.62
1:G:10:ILE:HG23	1:G:116:ILE:HG23	1.81	0.62
1:A:106:ALA:CA	1:A:111:ARG:HH12	2.13	0.62
1:A:469:VAL:O	1:A:472:ILE:HG23	2.00	0.62
1:D:337:LEU:O	1:D:341:LYS:HG3	1.99	0.62
1:D:356:ILE:O	1:D:362:VAL:HG21	1.99	0.62
1:D:430:ILE:HA	1:D:434:THR:CG2	2.30	0.62
1:E:122:THR:O	1:E:125:LEU:CD1	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:153:GLN:HG3	1:G:203:LYS:HD2	1.82	0.62
1:G:335:GLY:O	1:G:338:THR:HG22	2.00	0.62
1:B:106:ALA:HA	1:B:111:ARG:HH12	1.64	0.62
1:C:356:ILE:O	1:C:362:VAL:HG21	1.99	0.62
1:G:8:VAL:HG22	1:G:37:ILE:CG1	2.28	0.62
1:G:10:ILE:HG12	1:G:116:ILE:CG2	2.30	0.62
1:G:170:LEU:CD1	1:G:178:LEU:H	2.13	0.62
1:A:14:PRO:CG	1:A:93:LEU:HD22	2.28	0.62
1:A:19:LEU:HD13	1:A:23:LEU:HD13	1.82	0.62
1:E:155:PHE:O	1:E:159:ILE:HG23	2.00	0.62
1:F:148:LEU:HD12	1:F:198:TYR:OH	1.99	0.62
1:F:364:GLY:HA3	1:F:432:MET:HE3	1.82	0.62
1:G:4:SER:O	1:G:5:GLN:HB3	2.00	0.62
1:G:231:GLU:O	1:G:235:LEU:HD22	1.99	0.62
1:G:332:LEU:HD21	1:G:337:LEU:HD11	1.80	0.62
1:G:367:THR:HG23	1:G:369:CYS:N	2.13	0.62
1:A:193:GLN:O	1:A:196:GLU:CG	2.48	0.62
1:B:64:LYS:O	1:B:65:THR:OG1	2.12	0.62
1:B:356:ILE:O	1:B:362:VAL:HG21	2.00	0.62
1:C:37:ILE:HD12	1:C:65:THR:O	2.00	0.62
1:C:254:THR:HG21	1:C:352:ASN:ND2	2.14	0.62
1:C:371:TRP:HA	1:C:374:THR:HG23	1.81	0.62
1:E:356:ILE:O	1:E:362:VAL:HG21	1.99	0.62
1:F:396:ASN:O	1:F:400:LEU:HD12	1.99	0.62
1:G:268:ASN:C	1:G:269:GLU:HG2	2.20	0.62
1:G:474:SER:O	1:G:476:GLU:OE1	2.16	0.62
1:C:136:TYR:CE2	1:C:472:ILE:HD13	2.35	0.62
1:C:430:ILE:HA	1:C:434:THR:CG2	2.30	0.62
1:D:148:LEU:HD12	1:D:198:TYR:OH	2.00	0.62
1:D:367:THR:HG23	1:D:369:CYS:N	2.14	0.62
1:F:10:ILE:CG2	1:F:22:VAL:HG13	2.30	0.62
1:G:125:LEU:CG	1:G:126:PRO:HD3	2.29	0.62
1:A:292:TRP:O	1:A:296:LEU:CD1	2.40	0.61
1:E:159:ILE:HG21	1:E:190:ARG:HH22	1.65	0.61
1:E:183:VAL:HG21	1:E:187:LEU:CB	2.30	0.61
1:E:364:GLY:HA3	1:E:432:MET:CE	2.29	0.61
1:G:162:GLU:H	1:G:162:GLU:CD	2.03	0.61
1:A:133:ILE:N	1:A:133:ILE:HD12	2.15	0.61
1:A:159:ILE:C	1:A:159:ILE:HD12	2.21	0.61
1:C:76:ILE:HD11	1:C:93:LEU:HD22	1.82	0.61
1:C:246:PRO:HB2	1:C:375:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:435:LYS:HZ3	1:D:382:VAL:HG22	1.65	0.61
1:E:119:ILE:HG23	1:E:140:PRO:HD3	1.80	0.61
1:F:127:ILE:O	1:F:131:PHE:HD1	1.82	0.61
1:F:246:PRO:HB2	1:F:375:VAL:HG13	1.82	0.61
1:G:7:HIS:HD2	1:G:112:PRO:CA	1.98	0.61
1:G:52:GLU:O	1:G:56:LYS:HG3	2.01	0.61
1:G:125:LEU:HD12	1:G:126:PRO:N	2.16	0.61
1:B:10:ILE:CG2	1:B:22:VAL:HG13	2.30	0.61
1:B:291:ALA:C	1:B:295:GLU:OE1	2.39	0.61
1:D:55:LYS:HG3	1:D:56:LYS:HE3	1.83	0.61
1:E:220:GLU:O	1:E:224:ILE:HD12	2.00	0.61
1:F:426:GLY:O	1:F:430:ILE:HD12	1.99	0.61
1:G:356:ILE:O	1:G:362:VAL:HG21	2.00	0.61
1:E:151:TYR:CE2	1:E:154:VAL:CG2	2.83	0.61
1:F:143:ALA:N	1:F:213:ILE:HD11	2.16	0.61
1:G:176:LYS:HG2	1:G:177:ALA:N	2.15	0.61
1:C:350:TRP:CH2	2:C:501:U2F:O7'	2.52	0.61
1:C:429:ARG:NH1	1:D:260:ILE:CG2	2.63	0.61
1:E:18:HIS:O	1:E:22:VAL:CG1	2.49	0.61
1:G:434:THR:HG23	1:G:437:GLY:H	1.65	0.61
1:B:146:LEU:O	1:B:150:ILE:HD13	2.00	0.61
1:D:98:LEU:HA	1:D:101:ILE:HD12	1.80	0.61
1:F:133:ILE:HD13	1:F:133:ILE:N	2.15	0.61
1:G:165:GLU:H	1:G:165:GLU:CD	2.03	0.61
1:G:184:VAL:CG2	1:G:187:LEU:HD23	2.30	0.61
1:G:277:GLY:HA3	1:G:368:HIS:CE1	2.35	0.61
1:A:42:ILE:HA	1:A:71:VAL:HB	1.82	0.61
1:A:469:VAL:HA	1:A:472:ILE:HG23	1.83	0.61
1:E:97:ALA:O	1:E:101:ILE:HD12	2.01	0.61
1:A:148:LEU:HD12	1:A:198:TYR:OH	1.99	0.61
1:C:370:GLY:O	1:C:374:THR:HG22	2.00	0.61
1:G:61:ASN:HD21	1:G:66:ILE:H	1.48	0.61
1:G:165:GLU:OE2	1:G:166:LEU:HD22	2.00	0.61
1:G:249:ARG:NH2	2:G:501:U2F:O2'	2.34	0.61
1:G:290:LEU:CD2	1:G:294:LEU:HD11	2.31	0.61
1:A:54:LEU:C	1:A:54:LEU:HD12	2.20	0.61
1:C:239:VAL:HG13	1:C:240:PRO:HD2	1.83	0.61
1:A:33:HIS:CE1	1:A:465:ILE:CG1	2.83	0.61
1:A:131:PHE:N	1:A:131:PHE:CD1	2.68	0.61
1:E:61:ASN:OD1	1:E:64:LYS:N	2.34	0.60
1:A:50:GLU:CD	1:A:51:THR:HG23	2.20	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:ILE:CD1	1:B:440:ILE:CA	2.78	0.60
1:F:337:LEU:HD22	1:F:337:LEU:H	1.66	0.60
1:G:89:GLN:CA	1:G:92:LEU:CD2	2.70	0.60
1:G:332:LEU:CD2	1:G:337:LEU:HD11	2.31	0.60
1:C:72:PRO:HD2	1:C:100:LYS:CE	2.31	0.60
1:G:91:ARG:CZ	1:G:91:ARG:CA	2.73	0.60
1:G:472:ILE:CA	1:G:475:ARG:CZ	2.61	0.60
1:G:472:ILE:CG2	1:G:475:ARG:HH12	2.15	0.60
1:A:122:THR:HG21	1:A:201:LEU:HD22	1.83	0.60
1:A:356:ILE:O	1:A:362:VAL:HG21	2.01	0.60
1:B:396:ASN:O	1:B:400:LEU:HD12	2.00	0.60
1:D:290:LEU:HD23	1:D:294:LEU:HD11	1.83	0.60
1:B:115:LEU:CD2	1:B:117:VAL:HG12	2.32	0.60
1:B:383:PRO:HG2	1:B:431:LEU:HD11	1.82	0.60
1:G:294:LEU:CD1	1:G:294:LEU:N	2.65	0.60
1:A:262:TRP:CD2	1:A:345:LEU:HD13	2.36	0.60
1:A:277:GLY:O	1:A:306:ARG:NH2	2.34	0.60
1:B:90:LEU:O	1:B:94:VAL:HG23	2.02	0.60
1:B:292:TRP:O	1:B:295:GLU:HG2	2.01	0.60
1:F:254:THR:CG2	1:F:355:GLU:OE1	2.49	0.60
1:F:351:ALA:O	2:F:501:U2F:H8'	2.02	0.60
1:G:396:ASN:O	1:G:400:LEU:HD12	2.01	0.60
1:C:59:LEU:HD23	1:C:68:ILE:H	1.67	0.60
1:C:372:ASN:HB2	2:C:501:U2F:C1'	2.31	0.60
1:D:290:LEU:CD2	1:D:294:LEU:HD11	2.31	0.60
1:G:304:VAL:HA	1:G:347:VAL:HG23	1.83	0.60
1:C:136:TYR:CE2	1:C:472:ILE:CD1	2.85	0.60
1:C:220:GLU:O	1:C:224:ILE:HD12	2.02	0.60
1:A:24:VAL:CG2	1:A:247:LEU:HB3	2.32	0.60
1:A:201:LEU:HA	1:A:204:GLU:OE1	2.02	0.60
2:A:501:U2F:C6	3:A:502:T83:OAC	2.50	0.60
1:B:436:GLU:O	1:B:440:ILE:CD1	2.50	0.60
1:E:155:PHE:HZ	1:E:172:ILE:HD13	1.67	0.60
1:E:372:ASN:CB	2:E:501:U2F:O1A	2.45	0.60
1:F:154:VAL:HA	1:F:157:LYS:NZ	2.16	0.60
1:E:159:ILE:CG2	1:E:190:ARG:NH2	2.64	0.59
1:G:90:LEU:HD11	1:G:91:ARG:HH11	1.66	0.59
1:G:170:LEU:CD2	1:G:178:LEU:HB2	2.26	0.59
1:B:19:LEU:CD1	1:B:23:LEU:HD21	2.31	0.59
1:E:183:VAL:HG22	1:E:187:LEU:HB2	1.81	0.59
1:F:353:GLN:NE2	1:F:376:GLU:OE1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:190:ARG:HG3	1:G:195:TYR:CE2	2.37	0.59
1:A:396:ASN:O	1:A:400:LEU:HD12	2.02	0.59
1:C:71:VAL:HG23	1:C:100:LYS:CD	2.33	0.59
1:G:98:LEU:HD23	1:G:98:LEU:O	2.02	0.59
1:G:162:GLU:OE1	1:G:165:GLU:OE1	2.21	0.59
1:G:170:LEU:HD22	1:G:172:ILE:CD1	2.32	0.59
1:A:131:PHE:N	1:A:131:PHE:HD1	2.00	0.59
1:A:352:ASN:HB2	1:A:355:GLU:OE1	2.02	0.59
1:C:332:LEU:CD2	1:C:333:PRO:O	2.50	0.59
1:E:413:LEU:CD1	1:E:414:PRO:HD2	2.29	0.59
1:F:163:TYR:O	1:F:166:LEU:HG	2.02	0.59
1:G:127:ILE:HD13	1:G:128:ALA:H	1.66	0.59
1:G:170:LEU:HD12	1:G:171:LYS:H	1.67	0.59
1:G:472:ILE:HG22	1:G:475:ARG:HH12	1.68	0.59
1:C:430:ILE:HA	1:C:434:THR:HG23	1.83	0.59
2:C:501:U2F:PB	2:C:501:U2F:C4'	2.89	0.59
1:E:111:ARG:HG2	1:E:112:PRO:HD2	1.84	0.59
1:G:104:THR:HA	1:G:107:SER:OG	2.03	0.59
1:G:184:VAL:HG23	1:G:187:LEU:HD23	1.84	0.59
1:D:413:LEU:CD1	1:D:416:LYS:H	2.14	0.59
1:E:6:LEU:HD11	1:E:473:ARG:HH11	1.68	0.59
1:G:6:LEU:HD22	1:G:113:ASP:OD2	2.03	0.59
1:A:365:PHE:CE2	1:A:373:SER:OG	2.56	0.59
1:C:37:ILE:HD11	1:C:66:ILE:CA	2.31	0.59
1:E:9:ALA:HB3	1:E:115:LEU:HD13	1.83	0.59
1:E:79:LEU:N	1:E:79:LEU:HD12	2.17	0.59
1:F:273:PHE:HD1	1:F:274:VAL:N	2.01	0.59
1:C:396:ASN:O	1:C:400:LEU:HD12	2.02	0.59
1:A:160:GLU:H	1:A:160:GLU:CD	2.07	0.59
1:A:462:TYR:HA	1:A:465:ILE:CD1	2.33	0.59
1:C:14:PRO:N	1:C:42:ILE:CD1	2.64	0.59
1:E:108:MET:HE2	1:E:112:PRO:HD3	1.85	0.59
1:F:244:ILE:HD13	1:F:244:ILE:H	1.67	0.59
1:G:114:ALA:C	1:G:115:LEU:HD22	2.23	0.59
1:A:19:LEU:HD13	1:A:19:LEU:C	2.24	0.58
1:C:13:SER:HA	1:C:42:ILE:CD1	2.32	0.58
1:C:332:LEU:HD11	1:C:336:PHE:CD2	2.38	0.58
1:C:429:ARG:HH12	1:D:260:ILE:HG23	1.68	0.58
1:D:104:THR:O	1:D:108:MET:HG3	2.03	0.58
1:D:263:LEU:CB	1:D:359:HIS:HD1	2.15	0.58
1:D:413:LEU:HD13	1:D:413:LEU:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ILE:HG21	1:E:190:ARG:NH1	2.17	0.58
1:E:273:PHE:HD1	1:E:274:VAL:N	2.01	0.58
1:G:200:LYS:HD2	1:G:201:LEU:N	2.18	0.58
1:A:90:LEU:O	1:A:94:VAL:HG23	2.03	0.58
1:A:439:ARG:NH1	1:A:443:LYS:HE2	2.17	0.58
1:C:16:MET:CE	1:C:49:ALA:HB1	2.32	0.58
1:C:43:THR:HG22	1:C:71:VAL:O	2.03	0.58
1:C:95:ARG:HA	1:C:98:LEU:HD13	1.85	0.58
1:C:229:TYR:CE2	1:F:430:ILE:CD1	2.86	0.58
1:C:350:TRP:CH2	2:C:501:U2F:C7'	2.85	0.58
1:E:363:GLY:O	1:E:432:MET:HE2	2.03	0.58
1:E:428:VAL:O	1:E:431:LEU:O	2.21	0.58
1:G:101:ILE:HD11	1:G:127:ILE:CG2	2.30	0.58
1:B:105:ILE:HD13	1:B:127:ILE:HG21	1.85	0.58
1:B:285:LYS:NZ	1:B:288:THR:OG1	2.35	0.58
1:D:90:LEU:O	1:D:94:VAL:HG23	2.03	0.58
1:E:61:ASN:HD21	1:E:66:ILE:H	1.49	0.58
1:E:291:ALA:HB1	1:E:336:PHE:CE2	2.38	0.58
1:G:90:LEU:HD21	1:G:120:PHE:HB3	1.83	0.58
1:A:58:THR:HG22	1:A:59:LEU:HD12	1.86	0.58
1:A:172:ILE:CD1	1:A:175:CYS:O	2.46	0.58
1:B:89:GLN:O	1:B:93:LEU:HD23	2.03	0.58
1:D:413:LEU:HD22	1:D:414:PRO:CD	2.33	0.58
1:E:255:LEU:CG	1:E:256:ASN:H	2.16	0.58
1:G:26:GLY:HA2	1:G:29:LEU:CD2	2.27	0.58
1:G:294:LEU:CD1	1:G:294:LEU:H	2.16	0.58
1:C:437:GLY:HA2	1:C:440:ILE:HD12	1.86	0.58
1:D:273:PHE:HD1	1:D:274:VAL:N	2.02	0.58
1:G:55:LYS:HD2	1:G:55:LYS:C	2.23	0.58
1:A:55:LYS:HE3	1:A:55:LYS:O	2.03	0.58
1:A:163:TYR:O	1:A:166:LEU:HG	2.04	0.58
1:A:291:ALA:HB1	1:A:336:PHE:CE2	2.39	0.58
1:E:244:ILE:CG1	1:E:465:ILE:HG12	2.33	0.58
1:B:412:VAL:HG11	1:B:417:LYS:CE	2.34	0.58
1:C:352:ASN:HB2	1:C:355:GLU:OE1	2.04	0.58
1:D:45:THR:O	1:D:47:SER:N	2.36	0.58
1:F:239:VAL:CG2	1:F:240:PRO:HD2	2.33	0.58
1:G:155:PHE:CZ	1:G:172:ILE:HD13	2.37	0.58
1:B:392:GLU:CD	2:B:501:U2F:O4	2.41	0.58
1:C:231:GLU:O	1:C:235:LEU:HG	2.04	0.58
1:F:260:ILE:CG2	1:G:429:ARG:NH1	2.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:SER:HA	1:E:80:ILE:HD11	1.85	0.58
1:F:476:GLU:C	1:F:477:LEU:HD12	2.24	0.58
1:G:89:GLN:C	1:G:92:LEU:CD2	2.72	0.58
1:G:91:ARG:HE	1:G:200:LYS:HZ1	1.51	0.58
1:A:406:VAL:HG23	1:A:444:ALA:HB2	1.84	0.58
1:B:13:SER:HB3	1:B:14:PRO:HD2	1.86	0.58
1:E:53:PHE:HA	1:E:56:LYS:HD3	1.86	0.58
1:E:421:ARG:HA	1:E:424:ILE:CD1	2.34	0.58
1:G:133:ILE:HD13	1:G:133:ILE:N	2.19	0.58
1:C:433:GLN:NE2	1:D:359:HIS:NE2	2.50	0.57
1:D:290:LEU:HD23	1:D:294:LEU:CD1	2.34	0.57
1:G:101:ILE:C	1:G:101:ILE:HD12	2.24	0.57
1:D:263:LEU:CB	1:D:359:HIS:CE1	2.87	0.57
1:E:35:ILE:HG22	1:E:37:ILE:HD13	1.86	0.57
1:A:172:ILE:HD11	1:A:175:CYS:CA	2.34	0.57
1:B:109:THR:HG23	1:G:256:ASN:N	2.20	0.57
1:B:150:ILE:N	1:B:150:ILE:HD12	2.20	0.57
1:C:326:ARG:C	1:C:330:GLU:OE2	2.42	0.57
1:D:396:ASN:O	1:D:400:LEU:HD23	2.00	0.57
1:E:19:LEU:HD13	1:E:19:LEU:C	2.24	0.57
1:G:33:HIS:CB	1:G:35:ILE:HD11	2.34	0.57
1:G:249:ARG:HH21	1:G:354:VAL:HG13	1.69	0.57
1:B:98:LEU:HA	1:B:101:ILE:HG12	1.86	0.57
1:C:229:TYR:CD2	1:F:430:ILE:CD1	2.70	0.57
1:D:187:LEU:HD11	1:D:198:TYR:CE2	2.39	0.57
1:G:291:ALA:HB1	1:G:336:PHE:CE2	2.40	0.57
1:G:328:MET:CE	1:G:331:TYR:CE2	2.86	0.57
2:G:501:U2F:O1	2:G:501:U2F:O1A	2.22	0.57
1:B:239:VAL:HG23	1:B:240:PRO:CD	2.33	0.57
1:D:430:ILE:HA	1:D:434:THR:HG23	1.84	0.57
1:E:271:VAL:CG2	1:E:362:VAL:HA	2.32	0.57
1:G:55:LYS:HD2	1:G:56:LYS:N	2.19	0.57
1:G:200:LYS:HD2	1:G:200:LYS:C	2.24	0.57
1:E:430:ILE:HA	1:E:434:THR:HG21	1.85	0.57
1:A:101:ILE:HD11	1:A:127:ILE:HG12	1.87	0.57
1:A:249:ARG:NH2	1:A:354:VAL:HG23	2.19	0.57
1:E:263:LEU:CB	1:E:359:HIS:CE1	2.87	0.57
1:E:353:GLN:NE2	1:E:376:GLU:OE1	2.35	0.57
1:G:137:THR:HG23	1:G:208:PHE:CG	2.40	0.57
1:G:234:ARG:NH1	1:G:238:LYS:NZ	2.51	0.57
1:B:251:VAL:HG23	1:B:252:GLU:H	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ALA:HB1	1:D:336:PHE:CE2	2.39	0.57
1:F:60:THR:HG23	1:F:61:ASN:ND2	2.19	0.57
1:F:263:LEU:CB	1:F:359:HIS:HD1	2.17	0.57
1:G:98:LEU:C	1:G:98:LEU:CD2	2.72	0.57
1:B:328:MET:O	1:B:332:LEU:HD23	2.04	0.57
1:D:392:GLU:OE1	2:D:501:U2F:HC	2.04	0.57
1:E:299:GLN:HE22	1:E:433:GLN:NE2	2.03	0.57
1:F:151:TYR:CZ	1:F:154:VAL:HG21	2.37	0.57
1:F:239:VAL:HG23	1:F:240:PRO:CD	2.34	0.57
1:F:291:ALA:HB1	1:F:336:PHE:CE2	2.39	0.57
1:G:44:THR:OG1	1:G:46:SER:HB3	2.04	0.57
1:A:373:SER:HB2	2:A:501:U2F:O2A	2.05	0.57
1:A:439:ARG:HH11	1:A:443:LYS:HE2	1.70	0.57
1:B:216:TRP:O	1:B:219:LEU:O	2.23	0.57
1:C:408:ILE:HD12	1:C:430:ILE:HD11	1.86	0.57
1:D:429:ARG:O	1:D:433:GLN:CD	2.43	0.57
1:B:273:PHE:HD1	1:B:274:VAL:N	2.01	0.56
1:A:430:ILE:HA	1:A:434:THR:HG21	1.86	0.56
1:E:125:LEU:HD13	1:E:126:PRO:HD3	1.87	0.56
1:E:326:ARG:O	1:E:327:ASP:O	2.22	0.56
1:F:14:PRO:HG3	1:F:93:LEU:HD22	1.86	0.56
1:F:263:LEU:CB	1:F:359:HIS:CE1	2.87	0.56
1:G:49:ALA:O	1:G:51:THR:N	2.37	0.56
1:A:14:PRO:CD	1:A:42:ILE:HD11	2.36	0.56
1:A:20:ILE:HG12	1:A:21:PRO:CD	2.35	0.56
1:B:163:TYR:O	1:B:166:LEU:HG	2.05	0.56
1:B:428:VAL:O	1:B:431:LEU:O	2.23	0.56
1:C:297:SER:CB	1:C:428:VAL:HG21	2.35	0.56
1:C:419:VAL:O	1:C:420:LYS:HB2	2.05	0.56
1:E:35:ILE:HG22	1:E:37:ILE:CD1	2.36	0.56
1:F:224:ILE:C	1:F:224:ILE:HD13	2.25	0.56
1:F:449:LYS:O	1:F:453:ASN:OD1	2.23	0.56
1:G:10:ILE:HG22	1:G:22:VAL:HG12	1.87	0.56
1:G:231:GLU:O	1:G:235:LEU:CD2	2.54	0.56
1:G:251:VAL:HG12	1:G:252:GLU:N	2.21	0.56
1:G:387:TRP:CH2	1:G:424:ILE:HD11	2.40	0.56
1:G:10:ILE:CG2	1:G:22:VAL:HG12	2.36	0.56
1:A:50:GLU:CG	1:A:51:THR:N	2.67	0.56
1:A:139:HIS:CE1	1:A:142:THR:O	2.59	0.56
1:E:363:GLY:O	1:E:432:MET:CE	2.54	0.56
1:B:105:ILE:O	1:B:111:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD22	1:C:473:ARG:NH2	2.20	0.56
1:D:115:LEU:HD21	1:D:117:VAL:HG23	1.88	0.56
1:E:13:SER:HB3	1:E:14:PRO:HD2	1.86	0.56
1:F:286:GLN:NE2	1:F:419:VAL:HG22	2.16	0.56
1:G:328:MET:CE	1:G:331:TYR:HE2	2.19	0.56
1:G:442:GLU:O	1:G:446:LYS:HG2	2.06	0.56
1:A:374:THR:HA	1:A:384:MET:HE3	1.86	0.56
1:B:176:LYS:HE2	1:B:403:GLU:OE2	2.06	0.56
1:D:141:THR:HA	1:D:371:TRP:CD1	2.41	0.56
1:F:368:HIS:NE2	2:F:501:U2F:O2A	2.21	0.56
1:G:125:LEU:CD1	1:G:126:PRO:HD3	2.35	0.56
1:G:213:ILE:HD12	1:G:241:VAL:CG1	2.35	0.56
1:C:292:TRP:HB3	1:C:421:ARG:HG2	1.87	0.56
1:C:350:TRP:HH2	2:C:501:U2F:C7'	2.19	0.56
1:D:43:THR:O	1:D:44:THR:CB	2.54	0.56
1:F:469:VAL:HA	1:F:472:ILE:HD13	1.88	0.56
1:G:54:LEU:C	1:G:54:LEU:HD12	2.26	0.56
1:A:20:ILE:N	1:A:21:PRO:HD2	2.21	0.56
1:B:111:ARG:NH1	1:B:131:PHE:CE2	2.74	0.56
1:D:367:THR:O	1:D:386:ALA:O	2.24	0.56
1:G:141:THR:HA	1:G:371:TRP:CD1	2.41	0.56
1:G:193:GLN:O	1:G:195:TYR:N	2.39	0.56
1:G:254:THR:O	1:G:255:LEU:O	2.24	0.56
1:A:333:PRO:HG2	1:A:336:PHE:HD2	1.71	0.56
1:A:353:GLN:OE1	2:A:501:U2F:H2'	2.06	0.56
1:C:370:GLY:HA2	2:C:501:U2F:C4	2.34	0.56
1:E:244:ILE:HD12	1:E:461:SER:O	2.06	0.56
1:G:176:LYS:HE3	1:G:403:GLU:CG	2.36	0.56
1:B:53:PHE:O	1:B:57:THR:HG23	2.05	0.55
1:E:141:THR:HA	1:E:371:TRP:CD1	2.40	0.55
1:E:183:VAL:CG2	1:E:187:LEU:CB	2.82	0.55
1:F:76:ILE:HA	1:F:78:HIS:NE2	2.21	0.55
1:G:292:TRP:O	1:G:296:LEU:HD22	2.06	0.55
1:A:74:VAL:HG22	1:A:100:LYS:HE3	1.87	0.55
1:C:59:LEU:HD22	1:C:61:ASN:ND2	2.11	0.55
1:C:72:PRO:HD2	1:C:100:LYS:HZ1	1.69	0.55
1:C:87:PHE:HZ	1:C:201:LEU:HD22	1.71	0.55
1:C:435:LYS:NZ	1:D:382:VAL:CG2	2.68	0.55
1:E:74:VAL:HG22	1:E:75:ASP:O	2.06	0.55
1:E:244:ILE:HD13	1:E:465:ILE:HG12	1.82	0.55
1:E:251:VAL:HG23	1:E:354:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:ILE:H	1:F:172:ILE:HD12	1.71	0.55
1:A:328:MET:HA	1:A:331:TYR:CZ	2.41	0.55
1:B:54:LEU:O	1:B:58:THR:HG23	2.06	0.55
1:C:43:THR:HA	1:C:50:GLU:OE1	2.06	0.55
1:C:125:LEU:HD13	1:C:208:PHE:CE1	2.41	0.55
1:C:262:TRP:CG	1:C:345:LEU:HD22	2.42	0.55
1:C:330:GLU:CG	1:C:331:TYR:CD1	2.88	0.55
1:D:301:PHE:CE1	1:D:344:GLY:HA3	2.41	0.55
1:F:441:LYS:CG	1:F:445:LYS:NZ	2.70	0.55
1:G:139:HIS:CE1	1:G:142:THR:O	2.60	0.55
1:A:6:LEU:HB3	1:A:35:ILE:HD13	1.89	0.55
1:A:141:THR:HA	1:A:371:TRP:CD1	2.41	0.55
1:B:113:ASP:HA	1:B:133:ILE:HD11	1.88	0.55
1:B:148:LEU:HD22	1:B:178:LEU:CD1	2.37	0.55
1:D:429:ARG:CG	1:D:433:GLN:HE22	2.18	0.55
1:E:419:VAL:HG12	1:E:424:ILE:HG13	1.87	0.55
1:F:151:TYR:CD2	1:F:155:PHE:CE2	2.87	0.55
1:B:43:THR:O	1:B:73:SER:HB3	2.06	0.55
1:B:400:LEU:HA	1:B:404:LEU:CD1	2.37	0.55
1:B:440:ILE:HD12	1:B:440:ILE:CA	2.36	0.55
1:D:35:ILE:HG22	1:D:37:ILE:HD13	1.88	0.55
1:D:60:THR:HG23	1:D:61:ASN:O	2.06	0.55
1:D:251:VAL:HG12	1:D:354:VAL:HG12	1.88	0.55
1:E:277:GLY:HA3	1:E:368:HIS:CE1	2.42	0.55
1:F:35:ILE:HG22	1:F:37:ILE:HD13	1.88	0.55
1:F:474:SER:O	1:F:477:LEU:HD13	2.06	0.55
1:G:21:PRO:HA	1:G:24:VAL:HG12	1.89	0.55
1:G:36:LYS:HB2	1:G:65:THR:HA	1.88	0.55
1:G:112:PRO:HG2	1:G:115:LEU:HD21	1.88	0.55
1:C:89:GLN:O	1:C:93:LEU:HD23	2.06	0.55
1:C:141:THR:HA	1:C:371:TRP:CD1	2.41	0.55
1:F:76:ILE:HD11	1:F:79:LEU:HB3	1.89	0.55
1:G:105:ILE:HG23	1:G:108:MET:CE	2.36	0.55
1:B:141:THR:HA	1:B:371:TRP:CD1	2.42	0.55
1:B:295:GLU:CB	1:B:339:ARG:HH22	2.19	0.55
1:E:151:TYR:CD2	1:E:155:PHE:CE2	2.91	0.55
1:E:157:LYS:HG3	1:E:158:GLU:N	2.21	0.55
1:E:183:VAL:O	1:E:394:LYS:HE2	2.06	0.55
2:E:501:U2F:O1A	2:E:501:U2F:O3'	2.20	0.55
1:F:57:THR:O	1:F:60:THR:HG22	2.07	0.55
1:F:125:LEU:HD12	1:F:135:LYS:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:12:SER:HB3	1:G:41:ALA:HA	1.87	0.55
1:C:10:ILE:HG22	1:C:22:VAL:CG2	2.36	0.55
1:C:330:GLU:HG3	1:C:331:TYR:HD1	1.67	0.55
1:E:139:HIS:CE1	1:E:142:THR:O	2.59	0.55
1:E:214:ASN:O	1:E:245:GLY:HA3	2.07	0.55
1:F:19:LEU:O	1:F:23:LEU:HD12	2.06	0.55
1:A:272:LEU:C	1:A:272:LEU:HD12	2.26	0.55
1:C:9:ALA:HB3	1:C:115:LEU:HD12	1.87	0.55
1:E:88:THR:HG23	1:E:194:GLN:HG3	1.88	0.55
1:F:56:LYS:O	1:F:59:LEU:HD23	2.07	0.55
1:F:236:LEU:HD12	1:F:236:LEU:N	2.22	0.55
1:G:170:LEU:CG	1:G:178:LEU:H	2.19	0.55
1:A:10:ILE:CG2	1:A:22:VAL:HG13	2.37	0.55
1:A:442:GLU:O	1:A:446:LYS:HG3	2.06	0.55
1:C:19:LEU:HD13	1:C:19:LEU:C	2.27	0.55
1:C:328:MET:HE3	1:C:331:TYR:OH	2.07	0.55
1:A:73:SER:O	1:A:100:LYS:NZ	2.40	0.54
1:E:8:VAL:HG11	1:E:116:ILE:CD1	2.37	0.54
1:E:190:ARG:HG3	1:E:195:TYR:CE2	2.41	0.54
1:E:292:TRP:O	1:E:296:LEU:HD22	2.07	0.54
1:G:36:LYS:O	1:G:37:ILE:HD12	2.06	0.54
1:G:472:ILE:CA	1:G:475:ARG:HH12	2.07	0.54
1:A:6:LEU:HD21	1:A:473:ARG:HG2	1.89	0.54
1:A:433:GLN:C	1:A:433:GLN:CD	2.65	0.54
1:B:301:PHE:CE1	1:B:344:GLY:HA3	2.42	0.54
1:A:6:LEU:HG	1:A:472:ILE:CD1	2.35	0.54
1:C:20:ILE:N	1:C:21:PRO:HD2	2.23	0.54
1:E:155:PHE:CZ	1:E:172:ILE:HD13	2.43	0.54
1:F:14:PRO:CG	1:F:93:LEU:HD22	2.38	0.54
1:G:25:LEU:O	1:G:29:LEU:HD23	2.05	0.54
1:G:90:LEU:CD1	1:G:91:ARG:N	2.67	0.54
1:G:269:GLU:OE1	1:G:441:LYS:CE	2.55	0.54
1:G:353:GLN:OE1	2:G:501:U2F:H2'	2.06	0.54
1:B:329:SER:HA	1:B:332:LEU:HD23	1.89	0.54
1:C:43:THR:CG2	1:C:72:PRO:HA	2.37	0.54
1:E:48:SER:O	1:E:49:ALA:C	2.46	0.54
1:F:10:ILE:HG22	1:F:22:VAL:HG13	1.89	0.54
1:F:48:SER:O	1:F:49:ALA:C	2.45	0.54
1:G:90:LEU:HG	1:G:120:PHE:CD1	2.42	0.54
1:A:14:PRO:HG3	1:A:93:LEU:CD2	2.37	0.54
1:D:20:ILE:N	1:D:21:PRO:HD2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HD22	1:D:303:TRP:CH2	2.42	0.54
1:E:234:ARG:HH12	1:E:239:VAL:N	2.05	0.54
1:G:42:ILE:HD12	1:G:71:VAL:HB	1.89	0.54
1:G:53:PHE:HA	1:G:56:LYS:HG3	1.90	0.54
1:A:211:ILE:HD12	1:A:211:ILE:N	2.21	0.54
1:A:260:ILE:HD12	1:A:260:ILE:H	1.70	0.54
1:A:367:THR:HG21	1:A:384:MET:CE	2.37	0.54
1:B:137:THR:HG22	1:B:211:ILE:HG12	1.90	0.54
1:C:433:GLN:HG3	1:D:264:ASP:OD1	2.07	0.54
1:A:50:GLU:OE2	1:A:51:THR:CG2	2.45	0.54
1:C:121:CYS:O	1:C:124:ILE:CG1	2.49	0.54
1:D:102:HIS:HA	1:D:105:ILE:CD1	2.38	0.54
1:F:141:THR:HA	1:F:371:TRP:CD1	2.42	0.54
1:D:48:SER:O	1:D:49:ALA:C	2.45	0.54
1:D:95:ARG:HA	1:D:98:LEU:HD23	1.90	0.54
1:D:236:LEU:N	1:D:236:LEU:HD12	2.23	0.54
1:F:127:ILE:O	1:F:131:PHE:CD1	2.60	0.54
1:G:52:GLU:O	1:G:55:LYS:HG3	2.08	0.54
1:B:209:ASP:CG	1:B:475:ARG:HH12	2.12	0.54
1:C:178:LEU:HD11	1:C:183:VAL:HG12	1.89	0.54
1:C:262:TRP:CD1	1:C:345:LEU:HD13	2.42	0.54
1:C:298:GLN:NE2	1:D:255:LEU:HD23	2.23	0.54
1:D:115:LEU:CD2	1:D:117:VAL:HG23	2.38	0.54
1:D:257:ASP:O	1:D:258:GLU:HB2	2.07	0.54
1:E:255:LEU:H	1:E:255:LEU:CD2	2.21	0.54
1:E:442:GLU:O	1:E:446:LYS:HG2	2.08	0.54
1:G:90:LEU:HG	1:G:120:PHE:CG	2.43	0.54
1:G:170:LEU:CG	1:G:178:LEU:HB3	2.38	0.54
1:A:263:LEU:HB3	1:A:359:HIS:CD2	2.43	0.54
1:B:48:SER:O	1:B:49:ALA:C	2.46	0.54
1:C:13:SER:N	1:C:118:ASP:OD2	2.41	0.54
1:C:172:ILE:H	1:C:172:ILE:HD12	1.72	0.54
1:D:335:GLY:H	1:D:339:ARG:HH12	1.56	0.54
1:G:88:THR:O	1:G:92:LEU:CD1	2.56	0.54
1:A:277:GLY:HA3	1:A:368:HIS:CE1	2.42	0.53
1:B:101:ILE:HG13	1:B:124:ILE:HD12	1.89	0.53
1:B:172:ILE:HD12	1:B:175:CYS:HB2	1.90	0.53
1:D:43:THR:C	1:D:44:THR:HG22	2.21	0.53
1:E:219:LEU:HD12	1:E:220:GLU:HG3	1.90	0.53
1:E:383:PRO:CG	1:E:431:LEU:HD21	2.37	0.53
1:A:7:HIS:HD1	1:A:112:PRO:HA	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:O	1:A:49:ALA:C	2.47	0.53
1:A:468:LEU:O	1:A:472:ILE:HG22	2.07	0.53
1:B:297:SER:HB3	1:B:428:VAL:CG2	2.39	0.53
1:C:147:ALA:CA	1:C:150:ILE:HD11	2.28	0.53
1:D:292:TRP:C	1:D:296:LEU:HD12	2.27	0.53
1:F:98:LEU:HA	1:F:101:ILE:HG12	1.90	0.53
1:A:142:THR:OG1	1:A:145:THR:HG23	2.08	0.53
1:B:391:ALA:HB3	2:B:501:U2F:H6C2	1.90	0.53
1:D:10:ILE:HG22	1:D:22:VAL:CG1	2.38	0.53
1:E:112:PRO:HG2	1:E:115:LEU:HD21	1.90	0.53
1:E:139:HIS:CE1	1:E:141:THR:CG2	2.92	0.53
1:G:35:ILE:HD12	1:G:35:ILE:N	2.22	0.53
1:B:239:VAL:CG2	1:B:240:PRO:CD	2.87	0.53
1:E:19:LEU:CD1	1:E:23:LEU:HD13	2.35	0.53
1:G:6:LEU:HD13	1:G:113:ASP:OD1	2.08	0.53
1:G:352:ASN:O	1:G:356:ILE:HD12	2.07	0.53
1:A:260:ILE:HD12	1:A:260:ILE:N	2.23	0.53
1:D:184:VAL:HG12	1:D:392:GLU:HA	1.90	0.53
1:E:86:ILE:O	1:E:90:LEU:CD1	2.55	0.53
1:E:224:ILE:HA	1:E:227:LEU:HD12	1.91	0.53
1:F:224:ILE:HD13	1:F:225:ASN:N	2.23	0.53
1:G:105:ILE:O	1:G:106:ALA:HB3	2.08	0.53
1:G:466:CYS:O	1:G:470:LYS:HG2	2.08	0.53
1:A:21:PRO:HA	1:A:24:VAL:HG13	1.89	0.53
1:B:95:ARG:HA	1:B:98:LEU:HD23	1.91	0.53
1:D:413:LEU:CD1	1:D:416:LYS:N	2.70	0.53
1:E:142:THR:OG1	1:E:145:THR:HG23	2.09	0.53
1:F:264:ASP:OD1	1:G:433:GLN:NE2	2.42	0.53
1:A:273:PHE:HE2	1:A:353:GLN:HG3	1.73	0.53
1:B:110:HIS:CE1	1:G:255:LEU:HD23	2.43	0.53
1:G:90:LEU:HD13	1:G:91:ARG:CA	2.38	0.53
1:G:333:PRO:HG2	1:G:336:PHE:HD2	1.73	0.53
1:G:366:LEU:C	1:G:366:LEU:CD1	2.76	0.53
1:A:30:ALA:HA	1:A:35:ILE:O	2.09	0.53
1:B:33:HIS:CG	1:B:465:ILE:HG21	2.43	0.53
1:C:71:VAL:HG23	1:C:100:LYS:CE	2.39	0.53
2:C:501:U2F:H1	3:C:502:T83:OAC	2.09	0.53
1:D:335:GLY:N	1:D:339:ARG:HH12	2.06	0.53
1:E:263:LEU:CB	1:E:359:HIS:ND1	2.71	0.53
1:F:239:VAL:CG2	1:F:240:PRO:CD	2.87	0.53
1:F:260:ILE:HG22	1:G:429:ARG:HH12	1.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:263:LEU:CB	1:F:359:HIS:ND1	2.72	0.53
1:F:424:ILE:CD1	1:F:425:GLN:N	2.71	0.53
1:G:124:ILE:HG22	1:G:127:ILE:CD1	2.30	0.53
1:D:35:ILE:HG22	1:D:37:ILE:CD1	2.39	0.53
1:D:101:ILE:O	1:D:105:ILE:HD13	2.09	0.53
1:F:326:ARG:C	1:F:330:GLU:OE2	2.47	0.53
1:G:8:VAL:N	1:G:37:ILE:HD11	2.24	0.53
1:G:19:LEU:HD13	1:G:19:LEU:C	2.29	0.53
1:G:39:ILE:HG22	1:G:68:ILE:HA	1.91	0.53
1:G:197:GLU:HA	1:G:200:LYS:HG3	1.91	0.53
1:G:472:ILE:HA	1:G:475:ARG:NH2	2.21	0.53
1:B:422:GLU:O	1:B:425:GLN:HG3	2.09	0.53
1:C:370:GLY:O	1:C:374:THR:CG2	2.57	0.53
1:D:274:VAL:HG21	1:D:294:LEU:HD21	1.91	0.53
1:G:142:THR:OG1	1:G:145:THR:HG23	2.09	0.53
1:A:65:THR:O	1:A:66:ILE:O	2.27	0.52
1:B:110:HIS:CE1	1:G:255:LEU:CD2	2.93	0.52
1:F:328:MET:HA	1:F:331:TYR:CZ	2.44	0.52
1:F:364:GLY:HA3	1:F:432:MET:HE1	1.90	0.52
1:F:425:GLN:HE21	1:F:429:ARG:NE	2.06	0.52
1:G:296:LEU:HD13	1:G:296:LEU:N	2.25	0.52
1:A:33:HIS:NE2	1:A:465:ILE:CG1	2.72	0.52
1:A:179:ARG:NH2	1:A:402:GLU:OE2	2.35	0.52
1:C:48:SER:O	1:C:49:ALA:C	2.46	0.52
1:E:295:GLU:CD	1:E:339:ARG:NH1	2.63	0.52
1:G:26:GLY:O	1:G:29:LEU:HD23	2.09	0.52
1:G:52:GLU:O	1:G:56:LYS:HG2	2.08	0.52
1:G:127:ILE:HD13	1:G:128:ALA:CA	2.37	0.52
1:G:465:ILE:O	1:G:469:VAL:HG12	2.09	0.52
1:A:139:HIS:CE1	1:A:141:THR:OG1	2.63	0.52
1:A:401:THR:HG21	1:A:409:ARG:HD3	1.91	0.52
1:C:59:LEU:HD21	1:C:67:GLU:HG2	1.90	0.52
1:C:142:THR:OG1	1:C:145:THR:HG23	2.08	0.52
1:C:150:ILE:HD13	1:C:150:ILE:N	2.25	0.52
1:D:245:GLY:HA2	1:D:247:LEU:HD22	1.91	0.52
1:E:21:PRO:HA	1:E:24:VAL:HG12	1.91	0.52
1:F:188:LEU:HD23	1:F:188:LEU:H	1.74	0.52
1:G:76:ILE:HA	1:G:78:HIS:NE2	2.24	0.52
1:G:127:ILE:O	1:G:130:GLU:O	2.28	0.52
1:G:339:ARG:NH1	1:G:339:ARG:CG	2.63	0.52
1:A:272:LEU:C	1:A:272:LEU:CD1	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:GLU:O	1:A:454:ALA:O	2.27	0.52
1:B:10:ILE:HG22	1:B:22:VAL:HG13	1.92	0.52
1:B:297:SER:HB3	1:B:428:VAL:HG21	1.92	0.52
1:D:476:GLU:O	1:D:477:LEU:HB2	2.09	0.52
1:A:426:GLY:C	1:A:430:ILE:HD13	2.29	0.52
1:C:125:LEU:HD12	1:C:135:LYS:HD2	1.91	0.52
1:C:392:GLU:OE1	2:C:501:U2F:O6	2.28	0.52
1:E:244:ILE:HG12	1:E:465:ILE:HG12	1.91	0.52
1:F:20:ILE:HG21	1:F:249:ARG:HD2	1.92	0.52
1:F:200:LYS:O	1:F:204:GLU:HG3	2.09	0.52
1:G:151:TYR:CD1	1:G:154:VAL:CG2	2.90	0.52
1:G:236:LEU:N	1:G:236:LEU:HD12	2.25	0.52
1:E:33:HIS:CD2	1:E:465:ILE:HG21	2.44	0.52
1:E:166:LEU:HD12	1:E:168:GLU:H	1.74	0.52
1:F:35:ILE:HG22	1:F:37:ILE:CD1	2.39	0.52
1:F:381:GLY:N	1:F:448:LYS:HE3	2.25	0.52
1:A:16:MET:HA	1:A:19:LEU:HB3	1.92	0.52
1:B:64:LYS:C	1:B:65:THR:HG1	2.10	0.52
1:C:78:HIS:CE1	1:C:79:LEU:HG	2.45	0.52
1:D:102:HIS:HA	1:D:105:ILE:HD11	1.92	0.52
1:G:26:GLY:CA	1:G:29:LEU:CD2	2.88	0.52
1:G:97:ALA:HA	1:G:100:LYS:HE3	1.86	0.52
1:A:462:TYR:HD2	1:A:463:ASN:OD1	1.92	0.52
1:D:55:LYS:O	1:D:56:LYS:CG	2.47	0.52
1:E:166:LEU:HD12	1:E:168:GLU:HG2	1.91	0.52
1:E:326:ARG:C	1:E:327:ASP:O	2.49	0.52
1:F:9:ALA:O	1:F:115:LEU:HD12	2.09	0.52
1:A:106:ALA:O	1:A:107:SER:CB	2.57	0.52
1:A:108:MET:HB2	1:A:111:ARG:HD3	1.90	0.52
1:A:365:PHE:CZ	1:A:373:SER:OG	2.63	0.52
1:B:7:HIS:HD1	1:B:112:PRO:HA	1.75	0.52
1:D:142:THR:CG2	1:D:145:THR:HG23	2.40	0.52
1:F:430:ILE:CA	1:F:434:THR:HG23	2.31	0.52
1:G:328:MET:HE3	1:G:331:TYR:CZ	2.44	0.52
1:E:144:TRP:CH2	1:E:176:LYS:HD3	2.45	0.51
1:A:105:ILE:HA	1:A:108:MET:HG2	1.91	0.51
1:B:21:PRO:HA	1:B:24:VAL:HG13	1.91	0.51
1:B:434:THR:HG22	1:B:436:GLU:N	2.24	0.51
1:E:372:ASN:HD22	2:E:501:U2F:PA	2.32	0.51
1:F:43:THR:HG22	1:F:44:THR:H	1.76	0.51
1:F:154:VAL:HA	1:F:157:LYS:HZ1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:192:ASP:O	1:G:193:GLN:C	2.48	0.51
1:G:197:GLU:C	1:G:200:LYS:HG3	2.29	0.51
1:A:172:ILE:HG13	1:A:175:CYS:HB2	1.92	0.51
1:A:184:VAL:HG13	1:A:395:MET:CE	2.38	0.51
1:E:399:MET:HG2	1:E:404:LEU:CD2	2.40	0.51
1:G:19:LEU:HD13	1:G:23:LEU:CD2	2.40	0.51
1:G:80:ILE:HG13	1:G:84:THR:CB	2.40	0.51
1:C:175:CYS:HB3	1:C:223:THR:HG23	1.92	0.51
1:D:131:PHE:HB2	1:D:133:ILE:HD13	1.92	0.51
1:D:277:GLY:HA3	1:D:368:HIS:CE1	2.45	0.51
1:G:89:GLN:O	1:G:93:LEU:HD12	2.11	0.51
1:G:141:THR:CG2	1:G:371:TRP:HB2	2.28	0.51
1:G:366:LEU:C	1:G:366:LEU:HD13	2.31	0.51
1:B:166:LEU:O	1:B:167:LYS:CG	2.59	0.51
1:C:371:TRP:HA	1:C:374:THR:CG2	2.40	0.51
1:D:422:GLU:O	1:D:425:GLN:HG3	2.11	0.51
1:D:452:GLU:O	1:D:454:ALA:O	2.28	0.51
1:E:422:GLU:O	1:E:425:GLN:HG3	2.11	0.51
1:F:95:ARG:HA	1:F:98:LEU:HD23	1.92	0.51
1:F:392:GLU:OE2	2:F:501:U2F:O3	2.28	0.51
1:A:20:ILE:CG1	1:A:21:PRO:CD	2.89	0.51
1:B:293:GLY:HA3	1:B:424:ILE:CG1	2.41	0.51
1:C:72:PRO:HD2	1:C:100:LYS:NZ	2.25	0.51
1:C:350:TRP:HA	1:C:350:TRP:CE3	2.46	0.51
1:A:212:LEU:HD23	1:A:244:ILE:HD13	1.91	0.51
1:B:474:SER:HA	1:B:477:LEU:HG	1.93	0.51
2:C:501:U2F:O3A	2:C:501:U2F:C4'	2.58	0.51
1:E:255:LEU:H	1:E:255:LEU:HD22	1.75	0.51
1:G:419:VAL:HG12	1:G:424:ILE:HG12	1.93	0.51
1:A:429:ARG:HD2	1:A:433:GLN:HE21	1.75	0.51
1:C:297:SER:HB3	1:C:428:VAL:CG2	2.40	0.51
1:E:296:LEU:HD13	1:E:296:LEU:N	2.24	0.51
1:G:335:GLY:C	1:G:339:ARG:NH1	2.64	0.51
1:C:350:TRP:CH2	2:C:501:U2F:C8'	2.94	0.51
1:C:466:CYS:O	1:C:470:LYS:HG3	2.11	0.51
1:F:286:GLN:HE21	1:F:387:TRP:HZ2	1.58	0.51
1:A:122:THR:HG21	1:A:201:LEU:CD2	2.41	0.51
1:B:155:PHE:HB3	1:B:159:ILE:HD13	1.93	0.51
1:C:151:TYR:CD2	1:C:155:PHE:CE2	2.91	0.51
1:F:219:LEU:O	1:F:219:LEU:HD13	2.10	0.51
1:F:262:TRP:CD2	1:F:345:LEU:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ARG:NE	1:G:123:GLN:NE2	2.59	0.51
1:A:119:ILE:O	1:A:122:THR:HG22	2.11	0.50
1:B:254:THR:O	1:B:255:LEU:HG	2.10	0.50
1:B:377:SER:OG	1:B:384:MET:CE	2.59	0.50
1:C:42:ILE:HG22	1:C:101:ILE:HD11	1.93	0.50
1:C:126:PRO:O	1:C:129:GLU:HG3	2.11	0.50
1:E:274:VAL:HG21	1:E:294:LEU:HD21	1.92	0.50
1:F:333:PRO:HG2	1:F:336:PHE:HD2	1.76	0.50
2:F:501:U2F:O5	2:F:501:U2F:O1A	2.29	0.50
1:A:14:PRO:HG3	1:A:42:ILE:HD11	1.91	0.50
1:A:259:VAL:HG23	1:A:260:ILE:HD12	1.92	0.50
1:B:237:LEU:CD2	1:B:239:VAL:O	2.60	0.50
1:C:393:GLN:NE2	2:C:501:U2F:O3	2.44	0.50
1:G:146:LEU:HD21	1:G:211:ILE:HG21	1.93	0.50
1:A:131:PHE:HB2	1:A:133:ILE:CD1	2.38	0.50
1:B:142:THR:CG2	1:B:145:THR:HG23	2.41	0.50
1:C:43:THR:OG1	1:C:44:THR:N	2.44	0.50
1:C:178:LEU:HD13	1:C:183:VAL:HG12	1.92	0.50
1:D:209:ASP:CG	1:D:475:ARG:HH12	2.15	0.50
1:E:139:HIS:HE1	1:E:142:THR:O	1.93	0.50
1:E:159:ILE:HG22	1:E:190:ARG:HH22	1.71	0.50
1:F:142:THR:OG1	1:F:145:THR:HG23	2.11	0.50
1:G:99:PRO:HG2	1:G:100:LYS:NZ	2.26	0.50
1:A:367:THR:HG21	1:A:384:MET:HE1	1.92	0.50
1:A:410:PRO:N	1:A:427:MET:HE3	2.26	0.50
1:C:23:LEU:HD23	1:C:39:ILE:HD13	1.93	0.50
1:D:228:ARG:HA	1:D:234:ARG:HH21	1.76	0.50
1:D:413:LEU:HD12	1:D:416:LYS:HG3	1.92	0.50
1:A:78:HIS:CD2	1:A:79:LEU:HD12	2.46	0.50
1:A:101:ILE:O	1:A:105:ILE:HD12	2.11	0.50
1:A:139:HIS:HE1	1:A:142:THR:O	1.94	0.50
1:B:61:ASN:O	1:B:62:GLU:HG2	2.12	0.50
1:E:33:HIS:NE2	1:E:465:ILE:HG21	2.26	0.50
1:A:8:VAL:CG2	1:A:37:ILE:HG22	2.41	0.50
1:A:397:ALA:O	1:A:401:THR:HG23	2.12	0.50
1:C:88:THR:HG22	1:C:194:GLN:HA	1.94	0.50
1:D:10:ILE:HG21	1:D:22:VAL:HG12	1.93	0.50
1:E:333:PRO:HG2	1:E:336:PHE:HD2	1.76	0.50
1:F:237:LEU:HD12	1:F:239:VAL:H	1.77	0.50
1:F:372:ASN:HB2	2:F:501:U2F:O5'	2.12	0.50
1:B:88:THR:HG22	1:B:194:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:TRP:HA	1:B:295:GLU:OE2	2.09	0.50
1:C:13:SER:CA	1:C:42:ILE:CD1	2.89	0.50
1:C:50:GLU:O	1:C:54:LEU:HD13	2.12	0.50
1:C:185:ASP:HA	1:C:188:LEU:CD1	2.37	0.50
1:F:159:ILE:HD12	1:F:159:ILE:N	2.27	0.50
1:G:8:VAL:H	1:G:37:ILE:CD1	2.24	0.50
1:B:151:TYR:CD2	1:B:155:PHE:CE2	2.91	0.50
1:B:209:ASP:CG	1:B:475:ARG:NH1	2.65	0.50
1:D:419:VAL:HG12	1:D:424:ILE:HG13	1.93	0.50
1:F:418:LEU:HD13	1:F:418:LEU:C	2.32	0.50
1:B:353:GLN:OE1	2:B:501:U2F:H2'	2.12	0.50
1:D:53:PHE:O	1:D:57:THR:CG2	2.49	0.50
1:F:397:ALA:O	1:F:401:THR:HG23	2.12	0.50
1:B:393:GLN:HE21	2:B:501:U2F:H6C1	1.77	0.49
1:E:151:TYR:CD1	1:E:154:VAL:HG11	2.47	0.49
1:E:201:LEU:HD13	1:E:201:LEU:C	2.32	0.49
1:E:430:ILE:CA	1:E:434:THR:HG23	2.35	0.49
1:G:6:LEU:HD13	1:G:113:ASP:CG	2.32	0.49
1:G:237:LEU:HD12	1:G:239:VAL:H	1.77	0.49
1:D:248:ARG:HD3	1:D:379:THR:HG21	1.94	0.49
1:D:429:ARG:CA	1:D:433:GLN:OE1	2.56	0.49
1:E:237:LEU:HD12	1:E:239:VAL:H	1.77	0.49
1:F:154:VAL:CG2	1:F:155:PHE:H	2.25	0.49
1:A:274:VAL:HG21	1:A:294:LEU:HD21	1.94	0.49
1:B:251:VAL:HG23	1:B:252:GLU:N	2.26	0.49
1:B:274:VAL:HG21	1:B:294:LEU:HD21	1.93	0.49
1:D:33:HIS:NE2	1:D:465:ILE:HG21	2.26	0.49
1:D:173:PRO:HG3	1:D:232:LYS:HE3	1.94	0.49
1:D:352:ASN:HB3	1:D:355:GLU:OE1	2.11	0.49
1:D:396:ASN:ND2	1:D:396:ASN:N	2.60	0.49
1:E:397:ALA:O	1:E:401:THR:HG23	2.12	0.49
1:F:80:ILE:HG23	1:F:84:THR:CG2	2.43	0.49
1:F:150:ILE:HD13	1:F:237:LEU:CD2	2.42	0.49
1:F:290:LEU:HD13	1:F:303:TRP:CZ2	2.47	0.49
1:F:441:LYS:HG2	1:F:445:LYS:NZ	2.27	0.49
1:A:8:VAL:HG22	1:A:35:ILE:HD11	1.94	0.49
1:D:201:LEU:C	1:D:201:LEU:HD13	2.32	0.49
1:D:442:GLU:O	1:D:446:LYS:HG2	2.12	0.49
1:E:409:ARG:C	1:E:427:MET:HE3	2.33	0.49
1:F:326:ARG:HG2	1:F:331:TYR:HE2	1.76	0.49
1:G:127:ILE:CD1	1:G:128:ALA:N	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:VAL:CG1	1:G:252:GLU:H	2.22	0.49
1:G:470:LYS:O	1:G:472:ILE:O	2.30	0.49
1:C:332:LEU:CD1	1:C:336:PHE:CD2	2.96	0.49
1:E:457:ASP:HA	1:E:462:TYR:CD2	2.47	0.49
1:G:106:ALA:CA	1:G:108:MET:SD	2.99	0.49
1:A:248:ARG:HD3	1:A:379:THR:HG21	1.95	0.49
1:B:105:ILE:HG23	1:B:108:MET:HE3	1.93	0.49
1:C:13:SER:HA	1:C:42:ILE:HD12	1.93	0.49
1:E:363:GLY:C	1:E:432:MET:HE1	2.33	0.49
1:F:254:THR:HG23	1:F:355:GLU:OE1	2.11	0.49
1:G:4:SER:O	1:G:5:GLN:CB	2.59	0.49
1:A:439:ARG:NH1	1:A:443:LYS:CE	2.75	0.49
1:B:397:ALA:O	1:B:401:THR:HG23	2.12	0.49
1:D:106:ALA:HA	1:D:111:ARG:NH1	2.26	0.49
1:E:45:THR:HG23	1:E:73:SER:OG	2.12	0.49
1:E:78:HIS:CD2	1:E:79:LEU:CD1	2.96	0.49
1:E:309:SER:O	1:E:310:ASP:HB2	2.12	0.49
1:A:33:HIS:CE1	1:A:465:ILE:CD1	2.95	0.49
1:B:328:MET:C	1:B:332:LEU:HD23	2.33	0.49
1:B:387:TRP:CH2	1:B:419:VAL:HG21	2.46	0.49
1:E:328:MET:HE2	1:E:331:TYR:HE2	1.78	0.49
1:G:43:THR:OG1	1:G:44:THR:N	2.46	0.49
1:G:90:LEU:C	1:G:90:LEU:CD1	2.70	0.49
1:G:124:ILE:CG2	1:G:127:ILE:CD1	2.74	0.49
1:G:373:SER:HB3	2:G:501:U2F:O2A	2.12	0.49
1:D:52:GLU:O	1:D:55:LYS:O	2.29	0.49
1:D:88:THR:HG23	1:D:194:GLN:HB3	1.95	0.49
1:D:263:LEU:CB	1:D:359:HIS:ND1	2.71	0.49
1:D:372:ASN:ND2	2:D:501:U2F:O1A	2.45	0.49
1:G:62:GLU:HG2	1:G:63:GLU:OE1	2.13	0.49
1:G:170:LEU:HD11	1:G:178:LEU:N	2.24	0.49
2:G:501:U2F:F1	2:G:501:U2F:O5'	2.20	0.49
1:A:237:LEU:HD12	1:A:239:VAL:H	1.77	0.49
1:B:434:THR:O	1:B:438:LYS:HD2	2.12	0.49
1:C:147:ALA:CA	1:C:150:ILE:CD1	2.89	0.49
1:C:262:TRP:CZ3	1:C:266:GLN:CG	2.96	0.49
1:F:290:LEU:HD23	1:F:294:LEU:HD12	1.92	0.49
1:F:326:ARG:CG	1:F:331:TYR:HE2	2.26	0.49
1:G:52:GLU:O	1:G:55:LYS:HE3	2.12	0.49
1:G:335:GLY:O	1:G:339:ARG:NH1	2.46	0.49
1:G:336:PHE:N	1:G:339:ARG:HH12	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:469:VAL:HA	1:G:472:ILE:CG1	2.41	0.49
1:B:109:THR:HG23	1:G:255:LEU:CA	2.42	0.48
1:B:248:ARG:HD3	1:B:379:THR:HG21	1.95	0.48
1:B:258:GLU:HA	1:B:261:GLN:OE1	2.13	0.48
1:B:359:HIS:HB3	1:B:362:VAL:HG23	1.95	0.48
1:D:61:ASN:HB2	1:D:66:ILE:O	2.13	0.48
1:D:371:TRP:N	2:D:501:U2F:O4	2.39	0.48
1:F:387:TRP:CH2	1:F:419:VAL:HG21	2.48	0.48
1:G:200:LYS:HD3	1:G:204:GLU:OE2	2.13	0.48
1:G:284:THR:O	1:G:288:THR:HG23	2.13	0.48
1:G:466:CYS:HA	1:G:469:VAL:HG13	1.94	0.48
1:A:193:GLN:NE2	1:B:82:SER:OG	2.46	0.48
1:A:284:THR:O	1:A:288:THR:HG23	2.14	0.48
1:C:163:TYR:CE2	1:C:187:LEU:HD22	2.48	0.48
1:D:397:ALA:O	1:D:401:THR:HG23	2.13	0.48
1:E:74:VAL:CG2	1:E:75:ASP:N	2.76	0.48
1:E:76:ILE:HG13	1:E:93:LEU:HD23	1.96	0.48
1:B:201:LEU:HD13	1:B:201:LEU:C	2.32	0.48
1:C:59:LEU:CD2	1:C:68:ILE:N	2.76	0.48
1:C:476:GLU:OE1	1:C:476:GLU:HA	2.14	0.48
1:E:183:VAL:HG21	1:E:187:LEU:HB3	1.93	0.48
1:F:263:LEU:HD13	1:F:359:HIS:HD1	1.78	0.48
1:G:33:HIS:HB2	1:G:35:ILE:HD11	1.95	0.48
1:G:76:ILE:HA	1:G:78:HIS:CD2	2.48	0.48
1:G:183:VAL:O	1:G:394:LYS:CD	2.59	0.48
1:A:36:LYS:HB2	1:A:64:LYS:O	2.12	0.48
1:A:43:THR:OG1	1:A:44:THR:N	2.45	0.48
1:A:126:PRO:O	1:A:129:GLU:HG3	2.13	0.48
1:F:133:ILE:HA	1:F:475:ARG:NH2	2.29	0.48
1:G:29:LEU:HD23	1:G:29:LEU:N	2.26	0.48
1:A:14:PRO:HD3	1:A:42:ILE:HD11	1.94	0.48
1:A:425:GLN:HG3	1:A:426:GLY:N	2.27	0.48
1:B:109:THR:HG1	1:G:256:ASN:HA	1.74	0.48
1:B:175:CYS:SG	1:B:223:THR:HG23	2.53	0.48
1:B:285:LYS:HZ2	1:B:289:GLU:HG2	1.77	0.48
1:C:289:GLU:OE1	1:C:421:ARG:HG3	2.14	0.48
1:D:19:LEU:HD23	1:D:50:GLU:OE2	2.14	0.48
1:D:231:GLU:O	1:D:235:LEU:CD1	2.58	0.48
1:E:271:VAL:HG22	1:E:361:SER:C	2.30	0.48
1:E:305:VAL:HG11	1:E:346:VAL:CG1	2.44	0.48
1:F:21:PRO:O	1:F:24:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:430:ILE:HA	1:F:434:THR:HG21	1.91	0.48
1:G:111:ARG:O	1:G:111:ARG:HD2	2.12	0.48
1:G:117:VAL:HG23	1:G:118:ASP:O	2.14	0.48
1:C:21:PRO:O	1:C:24:VAL:HG22	2.12	0.48
1:E:159:ILE:HG21	1:E:190:ARG:NH2	2.25	0.48
1:F:131:PHE:HB2	1:F:133:ILE:HD12	1.94	0.48
1:G:64:LYS:HG3	1:G:65:THR:HG23	1.94	0.48
1:B:125:LEU:HD12	1:B:135:LYS:HD2	1.95	0.48
1:C:125:LEU:HD13	1:C:208:PHE:CD1	2.49	0.48
1:C:237:LEU:HD12	1:C:239:VAL:H	1.78	0.48
1:C:335:GLY:HA3	1:C:339:ARG:NH1	2.28	0.48
1:E:139:HIS:CE1	1:E:141:THR:HG22	2.49	0.48
1:F:264:ASP:OD1	1:G:433:GLN:HG3	2.14	0.48
1:G:269:GLU:OE1	1:G:441:LYS:HE3	2.14	0.48
1:A:33:HIS:NE2	1:A:465:ILE:HG12	2.28	0.48
1:A:88:THR:HG22	1:A:194:GLN:HA	1.96	0.48
1:A:184:VAL:CG1	1:A:395:MET:HE3	2.40	0.48
1:A:201:LEU:C	1:A:201:LEU:HD13	2.34	0.48
1:B:159:ILE:HD12	1:B:159:ILE:N	2.28	0.48
1:D:237:LEU:HD12	1:D:239:VAL:H	1.78	0.48
1:G:25:LEU:HD23	1:G:25:LEU:O	2.14	0.48
1:G:44:THR:OG1	1:G:46:SER:CB	2.62	0.48
1:E:94:VAL:O	1:E:97:ALA:N	2.46	0.48
1:E:151:TYR:CE1	1:E:154:VAL:HG11	2.49	0.48
1:B:284:THR:O	1:B:288:THR:HG23	2.14	0.48
1:B:409:ARG:C	1:B:427:MET:HE3	2.34	0.48
1:C:59:LEU:CD2	1:C:68:ILE:H	2.25	0.48
1:D:209:ASP:CG	1:D:475:ARG:NH1	2.67	0.48
1:G:248:ARG:HD3	1:G:379:THR:HG21	1.95	0.48
1:A:216:TRP:CH2	1:A:219:LEU:HD13	2.49	0.47
1:A:249:ARG:HB2	1:A:354:VAL:HG21	1.96	0.47
1:B:35:ILE:N	1:B:35:ILE:HD12	2.29	0.47
1:B:110:HIS:CD2	1:G:255:LEU:HA	2.49	0.47
1:C:359:HIS:HB3	1:C:362:VAL:HG23	1.96	0.47
1:E:75:ASP:C	1:E:76:ILE:HD13	2.35	0.47
1:G:404:LEU:N	1:G:404:LEU:HD12	2.28	0.47
1:C:213:ILE:HD12	1:C:241:VAL:CG2	2.42	0.47
1:C:284:THR:O	1:C:288:THR:HG23	2.14	0.47
1:E:8:VAL:CG1	1:E:116:ILE:CD1	2.92	0.47
1:E:162:GLU:OE2	1:E:190:ARG:HB3	2.15	0.47
1:F:305:VAL:HG11	1:F:346:VAL:CG1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:215:THR:OG1	1:G:219:LEU:HD23	2.14	0.47
1:G:273:PHE:HE2	1:G:353:GLN:HG3	1.79	0.47
1:G:387:TRP:CH2	1:G:424:ILE:CD1	2.97	0.47
1:G:410:PRO:N	1:G:427:MET:HE1	2.29	0.47
1:A:20:ILE:HG13	1:A:21:PRO:HD3	1.97	0.47
1:A:419:VAL:HG12	1:A:424:ILE:CD1	2.44	0.47
1:B:252:GLU:O	1:B:254:THR:HG23	2.14	0.47
1:B:420:LYS:O	1:B:424:ILE:HD13	2.14	0.47
1:C:297:SER:CB	1:C:428:VAL:CG2	2.93	0.47
1:C:436:GLU:HG3	1:C:439:ARG:HH22	1.79	0.47
1:E:163:TYR:OH	1:E:190:ARG:NH2	2.47	0.47
1:F:470:LYS:O	1:F:472:ILE:O	2.31	0.47
1:G:144:TRP:HA	1:G:223:THR:HG21	1.96	0.47
1:G:469:VAL:CA	1:G:472:ILE:HG12	2.42	0.47
1:B:44:THR:HG21	1:B:47:SER:HB3	1.97	0.47
1:B:112:PRO:O	1:B:133:ILE:CD1	2.62	0.47
1:B:117:VAL:HG23	1:B:118:ASP:O	2.15	0.47
1:D:18:HIS:O	1:D:22:VAL:HG23	2.11	0.47
1:D:43:THR:OG1	1:D:44:THR:N	2.47	0.47
1:D:162:GLU:O	1:D:166:LEU:HD23	2.13	0.47
1:D:263:LEU:HD13	1:D:359:HIS:HD1	1.79	0.47
1:D:305:VAL:HG11	1:D:346:VAL:CG1	2.44	0.47
1:E:12:SER:HB3	1:E:41:ALA:HA	1.97	0.47
1:F:284:THR:O	1:F:288:THR:HG23	2.14	0.47
1:G:170:LEU:HD13	1:G:171:LYS:N	2.26	0.47
1:A:51:THR:O	1:A:54:LEU:HG	2.15	0.47
1:B:7:HIS:HA	1:B:36:LYS:O	2.14	0.47
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.97	0.47
1:C:16:MET:HE2	1:C:49:ALA:HB1	1.96	0.47
1:C:112:PRO:O	1:C:133:ILE:CD1	2.62	0.47
1:C:215:THR:OG1	1:C:219:LEU:HD23	2.14	0.47
1:D:44:THR:HG21	1:D:47:SER:HB2	1.96	0.47
1:D:89:GLN:O	1:D:93:LEU:HD12	2.14	0.47
1:F:292:TRP:O	1:F:296:LEU:HD12	2.13	0.47
1:F:328:MET:HA	1:F:331:TYR:CE1	2.49	0.47
1:F:389:LEU:HD22	1:F:389:LEU:N	2.30	0.47
1:G:159:ILE:N	1:G:159:ILE:HD12	2.29	0.47
1:G:200:LYS:O	1:G:204:GLU:HG3	2.14	0.47
1:G:253:THR:HG23	1:G:253:THR:O	2.15	0.47
1:G:304:VAL:HG22	1:G:347:VAL:HG23	1.95	0.47
1:A:6:LEU:O	1:A:35:ILE:HD12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:HIS:HB3	1:A:362:VAL:HG23	1.97	0.47
1:B:109:THR:HG23	1:G:255:LEU:HA	1.95	0.47
1:B:329:SER:CA	1:B:332:LEU:HD23	2.44	0.47
1:B:440:ILE:CD1	1:B:440:ILE:H	2.28	0.47
1:D:98:LEU:CA	1:D:101:ILE:HD12	2.42	0.47
1:E:139:HIS:CE1	1:E:141:THR:HG23	2.50	0.47
1:G:53:PHE:HA	1:G:56:LYS:HE2	1.96	0.47
1:G:219:LEU:HD11	1:G:404:LEU:HD21	1.97	0.47
1:A:212:LEU:HD23	1:A:244:ILE:CD1	2.44	0.47
1:B:25:LEU:HD22	1:B:138:TYR:CD2	2.50	0.47
1:B:33:HIS:O	1:B:35:ILE:HD12	2.15	0.47
1:B:105:ILE:CD1	1:B:127:ILE:HG21	2.44	0.47
1:C:13:SER:HA	1:C:42:ILE:HD11	1.95	0.47
1:C:305:VAL:HG11	1:C:346:VAL:CG1	2.44	0.47
1:C:392:GLU:OE2	2:C:501:U2F:H4	2.14	0.47
1:C:429:ARG:HH12	1:D:260:ILE:HG22	1.77	0.47
1:D:12:SER:HB3	1:D:41:ALA:HA	1.95	0.47
1:D:151:TYR:CD2	1:D:155:PHE:CE2	2.91	0.47
1:D:284:THR:O	1:D:288:THR:HG23	2.13	0.47
1:E:101:ILE:O	1:E:105:ILE:HD12	2.14	0.47
1:E:290:LEU:HD21	1:E:294:LEU:HD11	1.92	0.47
1:E:325:THR:O	1:E:325:THR:HG22	2.15	0.47
1:F:14:PRO:HG3	1:F:93:LEU:CD2	2.45	0.47
1:F:16:MET:CE	1:F:53:PHE:CG	2.98	0.47
1:F:33:HIS:CE1	1:F:465:ILE:HG21	2.50	0.47
1:F:209:ASP:C	1:F:239:VAL:HG21	2.35	0.47
1:G:92:LEU:HD22	1:G:92:LEU:H	1.78	0.47
1:G:366:LEU:HD13	1:G:367:THR:N	2.30	0.47
1:G:372:ASN:HB2	2:G:501:U2F:O5'	2.14	0.47
1:A:210:GLY:HA2	1:A:239:VAL:HG23	1.97	0.47
1:A:253:THR:O	1:A:253:THR:HG22	2.14	0.47
1:A:278:SER:OG	2:A:501:U2F:O2B	2.31	0.47
1:A:353:GLN:HB2	2:A:501:U2F:C6'	2.45	0.47
1:C:71:VAL:HA	1:C:100:LYS:NZ	2.30	0.47
1:C:216:TRP:CH2	1:C:219:LEU:HD13	2.49	0.47
1:D:336:PHE:H	1:D:339:ARG:NH2	2.12	0.47
1:D:413:LEU:HD12	1:D:416:LYS:CG	2.45	0.47
1:E:249:ARG:HH22	2:E:501:U2F:H3	1.62	0.47
1:A:33:HIS:C	1:A:35:ILE:H	2.18	0.47
1:A:63:GLU:N	1:A:65:THR:HG22	2.29	0.47
1:B:95:ARG:CZ	1:B:96:GLU:OE2	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:434:THR:HG22	1:B:436:GLU:H	1.80	0.47
1:D:292:TRP:CG	1:D:421:ARG:NH1	2.83	0.47
1:E:27:ASN:HA	1:E:66:ILE:HD11	1.97	0.47
1:E:108:MET:CE	1:E:112:PRO:HD3	2.45	0.47
1:F:224:ILE:HD11	1:F:228:ARG:NE	2.30	0.47
1:G:216:TRP:CH2	1:G:219:LEU:HD13	2.49	0.47
1:A:73:SER:C	1:A:100:LYS:HZ1	2.19	0.47
1:A:215:THR:OG1	1:A:219:LEU:HD23	2.15	0.47
1:B:56:LYS:O	1:B:59:LEU:HD23	2.15	0.47
1:C:104:THR:O	1:C:108:MET:HG3	2.14	0.47
1:C:433:GLN:O	1:D:360:SER:HB3	2.15	0.47
1:D:39:ILE:CD1	1:D:39:ILE:CG2	2.93	0.47
1:D:359:HIS:HB3	1:D:362:VAL:HG23	1.96	0.47
1:G:18:HIS:O	1:G:22:VAL:HG23	2.14	0.47
1:G:101:ILE:HG13	1:G:102:HIS:N	2.30	0.47
1:A:62:GLU:HB2	1:A:66:ILE:CD1	2.45	0.46
1:A:105:ILE:O	1:A:106:ALA:CB	2.62	0.46
1:A:292:TRP:CG	1:A:421:ARG:NH1	2.83	0.46
1:B:114:ALA:CB	1:B:472:ILE:HD12	2.46	0.46
1:C:135:LYS:NZ	1:C:209:ASP:OD1	2.48	0.46
1:C:248:ARG:HD2	1:C:379:THR:HG21	1.96	0.46
1:C:421:ARG:O	1:C:424:ILE:N	2.48	0.46
1:D:184:VAL:CG2	1:D:187:LEU:HD13	2.44	0.46
1:D:215:THR:OG1	1:D:219:LEU:HD23	2.15	0.46
1:F:21:PRO:HA	1:F:24:VAL:CG2	2.44	0.46
1:G:105:ILE:HG23	1:G:108:MET:HE3	1.97	0.46
1:G:328:MET:CE	1:G:331:TYR:OH	2.63	0.46
1:A:409:ARG:C	1:A:427:MET:HE3	2.35	0.46
1:B:215:THR:OG1	1:B:219:LEU:HD23	2.14	0.46
1:C:257:ASP:OD2	1:C:260:ILE:HD13	2.14	0.46
1:C:435:LYS:HZ3	1:D:382:VAL:CG2	2.27	0.46
1:D:175:CYS:SG	1:D:223:THR:HG23	2.55	0.46
1:D:200:LYS:HE2	1:D:200:LYS:HA	1.97	0.46
1:D:353:GLN:OE1	2:D:501:U2F:H2'	2.16	0.46
1:D:418:LEU:CD1	1:D:418:LEU:C	2.83	0.46
1:F:183:VAL:HG23	1:F:188:LEU:HD22	1.98	0.46
1:F:276:PHE:CE2	1:F:282:LEU:HD21	2.49	0.46
1:F:475:ARG:HD2	1:F:475:ARG:C	2.35	0.46
1:G:74:VAL:HG13	1:G:100:LYS:CE	2.43	0.46
1:G:91:ARG:O	1:G:91:ARG:NH2	2.49	0.46
1:G:190:ARG:HG3	1:G:195:TYR:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:MET:C	1:A:18:HIS:N	2.67	0.46
1:A:20:ILE:HD11	2:A:501:U2F:H4'	1.96	0.46
1:A:92:LEU:CD2	1:B:81:ASN:ND2	2.70	0.46
1:C:332:LEU:CD1	1:C:336:PHE:HB3	2.43	0.46
1:D:216:TRP:CH2	1:D:219:LEU:HD13	2.50	0.46
1:E:119:ILE:HG22	1:E:139:HIS:HA	1.98	0.46
1:G:90:LEU:HD13	1:G:91:ARG:HH11	1.76	0.46
1:A:61:ASN:HB3	1:A:67:GLU:OE1	2.15	0.46
1:B:61:ASN:C	1:B:62:GLU:HG2	2.35	0.46
1:B:435:LYS:O	1:B:439:ARG:HD2	2.15	0.46
1:C:25:LEU:HD22	1:C:138:TYR:CD2	2.50	0.46
1:C:33:HIS:O	1:C:35:ILE:HD12	2.15	0.46
1:E:153:GLN:NE2	1:E:236:LEU:HD12	2.30	0.46
1:E:359:HIS:HB3	1:E:362:VAL:HG23	1.96	0.46
1:F:117:VAL:HG23	1:F:118:ASP:O	2.16	0.46
1:G:123:GLN:OE1	1:G:123:GLN:N	2.44	0.46
1:A:8:VAL:N	1:A:35:ILE:HD11	2.30	0.46
1:B:410:PRO:N	1:B:427:MET:HE3	2.30	0.46
1:C:350:TRP:CZ2	2:C:501:U2F:C7'	2.98	0.46
1:F:16:MET:HE1	1:F:53:PHE:CG	2.51	0.46
1:F:40:LEU:HD12	1:F:69:ILE:HB	1.97	0.46
1:B:209:ASP:C	1:B:239:VAL:HG21	2.35	0.46
1:B:277:GLY:HA3	1:B:368:HIS:CE1	2.51	0.46
1:B:295:GLU:CG	1:B:339:ARG:HH22	2.29	0.46
1:C:10:ILE:HG22	1:C:22:VAL:HG23	1.97	0.46
1:C:248:ARG:HG2	1:C:375:VAL:HG12	1.97	0.46
1:E:14:PRO:HG3	1:E:93:LEU:HD12	1.97	0.46
1:F:183:VAL:HG23	1:F:188:LEU:CD2	2.45	0.46
1:F:441:LYS:HG2	1:F:445:LYS:CE	2.46	0.46
1:G:43:THR:CG2	1:G:72:PRO:HA	2.46	0.46
1:A:248:ARG:HH12	1:A:354:VAL:CG1	2.28	0.46
1:B:12:SER:HB3	1:B:41:ALA:HA	1.97	0.46
1:B:44:THR:CG2	1:B:47:SER:HB3	2.45	0.46
1:C:12:SER:HB3	1:C:41:ALA:HA	1.97	0.46
1:C:180:PRO:O	1:C:183:VAL:HG13	2.16	0.46
1:C:328:MET:SD	1:C:348:PRO:HB3	2.56	0.46
1:C:332:LEU:HD11	1:C:336:PHE:HD2	1.80	0.46
1:D:55:LYS:NZ	1:D:55:LYS:HB3	2.30	0.46
1:D:261:GLN:C	1:D:262:TRP:O	2.48	0.46
1:D:333:PRO:HG2	1:D:336:PHE:HD2	1.81	0.46
1:F:125:LEU:HB3	1:F:126:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:HIS:ND1	1:G:18:HIS:N	2.64	0.46
1:G:297:SER:N	1:G:425:GLN:HG3	2.31	0.46
1:A:78:HIS:CD2	1:A:79:LEU:CD1	2.99	0.46
1:B:105:ILE:HD13	1:B:127:ILE:CG2	2.45	0.46
1:B:141:THR:HG21	1:B:392:GLU:OE2	2.16	0.46
1:B:216:TRP:CH2	1:B:219:LEU:HD13	2.50	0.46
1:B:353:GLN:OE1	1:B:376:GLU:OE1	2.34	0.46
1:C:37:ILE:HD13	1:C:37:ILE:C	2.36	0.46
1:E:19:LEU:HD11	1:E:53:PHE:HE2	1.80	0.46
1:F:328:MET:HE3	1:F:348:PRO:HG3	1.98	0.46
1:G:54:LEU:HD12	1:G:55:LYS:N	2.31	0.46
1:G:100:LYS:O	1:G:104:THR:HG22	2.15	0.46
1:G:329:SER:HA	1:G:332:LEU:HD21	1.98	0.46
1:A:33:HIS:HE1	1:A:465:ILE:HD11	1.79	0.46
1:D:36:LYS:C	1:D:37:ILE:HD13	2.37	0.46
1:D:187:LEU:HD11	1:D:198:TYR:CD2	2.50	0.46
1:E:24:VAL:HG21	1:E:248:ARG:N	2.30	0.46
1:E:33:HIS:O	1:E:35:ILE:HD12	2.16	0.46
1:E:119:ILE:HG23	1:E:140:PRO:CD	2.44	0.46
1:E:373:SER:HG	2:E:501:U2F:H5'2	1.77	0.46
1:F:25:LEU:HD22	1:F:138:TYR:CD2	2.50	0.46
1:F:388:PRO:C	1:F:389:LEU:HD22	2.36	0.46
1:G:76:ILE:HB	1:G:96:GLU:OE1	2.15	0.46
1:A:143:ALA:HB2	1:A:213:ILE:HD12	1.96	0.46
1:A:193:GLN:O	1:A:196:GLU:HG3	2.16	0.46
1:B:19:LEU:HD12	1:B:23:LEU:HD22	1.94	0.46
1:B:440:ILE:HD12	1:B:440:ILE:H	1.81	0.46
2:C:501:U2F:O2B	2:C:501:U2F:H5'2	2.16	0.46
2:E:501:U2F:O6'	2:E:501:U2F:C2'	2.64	0.46
1:F:33:HIS:O	1:F:35:ILE:HD12	2.16	0.46
1:G:10:ILE:CD1	1:G:25:LEU:HD22	2.40	0.46
1:G:192:ASP:O	1:G:194:GLN:N	2.49	0.46
1:A:455:LEU:HD12	1:A:461:SER:OG	2.15	0.45
1:B:10:ILE:HG21	1:B:22:VAL:HG13	1.98	0.45
1:B:399:MET:HG2	1:B:404:LEU:HD11	1.98	0.45
1:C:409:ARG:C	1:C:427:MET:HE3	2.36	0.45
1:D:43:THR:OG1	1:D:72:PRO:HA	2.16	0.45
1:D:88:THR:HG22	1:D:194:GLN:HA	1.97	0.45
1:D:95:ARG:HD3	1:D:123:GLN:CD	2.37	0.45
1:E:259:VAL:HA	1:E:345:LEU:HD21	1.98	0.45
1:F:180:PRO:O	1:F:183:VAL:HG13	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:PHE:CA	1:G:56:LYS:HG3	2.46	0.45
1:G:175:CYS:SG	1:G:223:THR:HG23	2.56	0.45
1:A:52:GLU:OE1	1:A:53:PHE:N	2.49	0.45
1:B:180:PRO:O	1:B:183:VAL:HG13	2.16	0.45
1:C:95:ARG:CA	1:C:98:LEU:HD13	2.46	0.45
1:C:125:LEU:HB3	1:C:126:PRO:HD3	1.97	0.45
1:D:33:HIS:O	1:D:35:ILE:HD12	2.16	0.45
1:D:45:THR:O	1:D:45:THR:HG23	2.16	0.45
1:E:117:VAL:HG23	1:E:118:ASP:O	2.15	0.45
1:G:193:GLN:O	1:G:196:GLU:N	2.49	0.45
1:A:12:SER:HB3	1:A:41:ALA:HA	1.98	0.45
1:A:222:GLU:OE2	1:A:223:THR:OG1	2.34	0.45
1:B:187:LEU:HD11	1:B:198:TYR:CE2	2.51	0.45
1:B:249:ARG:NH1	2:B:501:U2F:O2'	2.49	0.45
1:D:95:ARG:HD3	1:D:123:GLN:HE22	1.80	0.45
1:D:163:TYR:HA	1:D:166:LEU:HD21	1.97	0.45
1:E:364:GLY:N	1:E:432:MET:HE1	2.31	0.45
1:F:36:LYS:C	1:F:37:ILE:HD13	2.36	0.45
1:F:274:VAL:HG21	1:F:294:LEU:HD21	1.97	0.45
1:G:125:LEU:N	1:G:126:PRO:HD2	2.31	0.45
1:G:139:HIS:HE1	1:G:142:THR:O	1.98	0.45
1:A:101:ILE:CD1	1:A:127:ILE:HG12	2.47	0.45
1:A:374:THR:HG22	1:A:384:MET:HE1	1.98	0.45
1:B:50:GLU:O	1:B:54:LEU:CD1	2.65	0.45
1:C:427:MET:HA	1:C:430:ILE:HG12	1.99	0.45
1:D:46:SER:HA	1:D:51:THR:HG21	1.98	0.45
1:D:72:PRO:O	1:D:73:SER:HB3	2.17	0.45
1:E:36:LYS:C	1:E:37:ILE:HD13	2.36	0.45
1:F:25:LEU:CD1	1:F:29:LEU:HD11	2.47	0.45
1:G:119:ILE:O	1:G:122:THR:HG23	2.15	0.45
1:G:166:LEU:HD12	1:G:168:GLU:H	1.81	0.45
1:A:65:THR:HG23	1:A:66:ILE:HG23	1.98	0.45
1:A:430:ILE:CA	1:A:434:THR:HG23	2.35	0.45
1:A:472:ILE:HD13	1:A:472:ILE:C	2.36	0.45
1:B:332:LEU:HD22	1:B:332:LEU:N	2.31	0.45
1:C:435:LYS:HE3	1:D:359:HIS:O	2.16	0.45
1:C:436:GLU:HG3	1:C:439:ARG:NH2	2.31	0.45
1:E:114:ALA:O	1:E:115:LEU:HD22	2.17	0.45
1:E:176:LYS:CE	1:E:403:GLU:OE1	2.65	0.45
1:E:372:ASN:HB2	2:E:501:U2F:PA	2.57	0.45
1:F:352:ASN:O	1:F:356:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:HIS:CE1	1:G:79:LEU:HB2	2.52	0.45
1:B:372:ASN:HA	1:B:375:VAL:CG2	2.47	0.45
1:C:133:ILE:HG22	1:C:134:SER:O	2.16	0.45
1:D:180:PRO:O	1:D:183:VAL:HG13	2.17	0.45
1:E:413:LEU:HD12	1:E:414:PRO:CD	2.41	0.45
1:G:8:VAL:H	1:G:37:ILE:HD11	1.80	0.45
1:G:90:LEU:HD13	1:G:91:ARG:HA	1.98	0.45
1:A:141:THR:HG21	1:A:392:GLU:OE2	2.17	0.45
1:C:260:ILE:HD12	1:C:260:ILE:N	2.32	0.45
1:F:141:THR:HG21	1:F:392:GLU:OE2	2.17	0.45
1:F:474:SER:O	1:F:477:LEU:HD11	2.17	0.45
1:B:42:ILE:CD1	1:B:94:VAL:HG13	2.47	0.45
1:B:110:HIS:NE2	1:G:255:LEU:CG	2.76	0.45
1:B:187:LEU:HD11	1:B:198:TYR:CD2	2.52	0.45
1:C:50:GLU:O	1:C:54:LEU:CD1	2.65	0.45
1:C:68:ILE:C	1:C:69:ILE:HD13	2.37	0.45
1:C:101:ILE:O	1:C:105:ILE:HD12	2.15	0.45
1:C:383:PRO:HB2	1:C:431:LEU:HD11	1.99	0.45
1:D:184:VAL:HG12	1:D:392:GLU:CA	2.47	0.45
1:E:37:ILE:HD13	1:E:37:ILE:N	2.32	0.45
1:G:146:LEU:HD22	1:G:205:TYR:CE2	2.52	0.45
1:G:305:VAL:CG1	1:G:346:VAL:HG13	2.47	0.45
1:G:359:HIS:HB3	1:G:362:VAL:HG23	1.98	0.45
1:A:63:GLU:C	1:A:65:THR:N	2.70	0.45
1:B:144:TRP:HA	1:B:223:THR:HG21	1.99	0.45
1:C:148:LEU:HD12	1:C:148:LEU:O	2.16	0.45
1:E:104:THR:O	1:E:108:MET:HG3	2.17	0.45
1:E:190:ARG:HG3	1:E:195:TYR:CD2	2.51	0.45
1:E:231:GLU:HG2	1:E:232:LYS:N	2.32	0.45
1:E:383:PRO:HG2	1:E:431:LEU:HD21	1.98	0.45
1:F:383:PRO:HB2	1:F:431:LEU:HD11	1.99	0.45
1:G:113:ASP:O	1:G:114:ALA:CB	2.64	0.45
1:A:263:LEU:CB	1:A:359:HIS:CD2	3.00	0.45
1:A:305:VAL:HG11	1:A:346:VAL:CG1	2.46	0.45
1:B:424:ILE:O	1:B:428:VAL:HG22	2.17	0.45
1:B:442:GLU:O	1:B:446:LYS:HD3	2.17	0.45
1:C:146:LEU:C	1:C:146:LEU:HD23	2.37	0.45
1:C:425:GLN:O	1:C:428:VAL:HG22	2.17	0.45
1:C:466:CYS:HA	1:C:469:VAL:HG22	1.99	0.45
1:D:117:VAL:HG11	1:D:121:CYS:C	2.37	0.45
1:E:250:LYS:HD3	1:E:250:LYS:HA	1.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:286:GLN:NE2	1:F:387:TRP:HZ2	2.15	0.45
1:G:264:ASP:OD1	1:G:359:HIS:CE1	2.70	0.45
1:A:175:CYS:SG	1:A:223:THR:HG23	2.56	0.44
1:C:401:THR:HG21	1:C:409:ARG:HD3	1.99	0.44
1:D:35:ILE:HD12	1:D:35:ILE:N	2.32	0.44
1:D:109:THR:HG22	1:D:110:HIS:CD2	2.53	0.44
1:D:150:ILE:HD13	1:D:237:LEU:HD23	1.98	0.44
1:E:61:ASN:HD21	1:E:66:ILE:N	2.10	0.44
1:E:119:ILE:CG2	1:E:140:PRO:HD2	2.47	0.44
1:F:127:ILE:HG23	1:F:131:PHE:CE1	2.52	0.44
1:F:328:MET:CE	1:F:346:VAL:HG12	2.47	0.44
1:G:62:GLU:CG	1:G:63:GLU:OE1	2.65	0.44
1:G:90:LEU:HD13	1:G:91:ARG:NH1	2.32	0.44
1:G:377:SER:HB2	1:G:382:VAL:HG23	1.99	0.44
1:A:44:THR:HG21	1:A:47:SER:OG	2.17	0.44
1:B:412:VAL:HG11	1:B:417:LYS:HB3	1.99	0.44
1:C:41:ALA:O	1:C:71:VAL:CG1	2.63	0.44
1:C:294:LEU:N	1:C:294:LEU:CD2	2.80	0.44
1:D:150:ILE:HD13	1:D:237:LEU:CD2	2.47	0.44
1:E:50:GLU:O	1:E:54:LEU:CD2	2.63	0.44
1:G:38:THR:HB	1:G:67:GLU:CG	2.47	0.44
1:G:353:GLN:OE1	1:G:376:GLU:OE1	2.36	0.44
1:A:130:GLU:C	1:A:131:PHE:CD1	2.91	0.44
1:C:146:LEU:HD12	1:C:213:ILE:HG21	1.99	0.44
1:C:327:ASP:O	1:C:330:GLU:HG2	2.16	0.44
1:E:119:ILE:HD11	1:E:120:PHE:CZ	2.53	0.44
1:G:29:LEU:HB2	1:G:35:ILE:HD13	1.99	0.44
1:G:187:LEU:N	1:G:187:LEU:CD2	2.80	0.44
2:G:501:U2F:O6	2:G:501:U2F:H1	2.17	0.44
1:A:126:PRO:HG2	1:A:127:ILE:HD13	1.98	0.44
1:C:21:PRO:HA	1:C:24:VAL:HG22	2.00	0.44
1:G:29:LEU:CD2	1:G:29:LEU:H	2.28	0.44
1:G:234:ARG:NH1	1:G:238:LYS:HZ3	2.15	0.44
1:B:109:THR:HA	1:G:255:LEU:O	2.18	0.44
1:B:272:LEU:CD2	1:B:428:VAL:HG12	2.48	0.44
1:D:234:ARG:HA	1:D:234:ARG:HD3	1.88	0.44
1:E:246:PRO:CD	1:E:455:LEU:HD11	2.48	0.44
1:G:116:ILE:HD12	1:G:117:VAL:N	2.33	0.44
1:G:166:LEU:O	1:G:167:LYS:HB3	2.17	0.44
1:A:249:ARG:NH2	2:A:501:U2F:O6'	2.51	0.44
1:C:16:MET:N	1:C:16:MET:SD	2.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:110:HIS:O	1:C:111:ARG:O	2.35	0.44
1:C:222:GLU:HG2	1:C:223:THR:N	2.32	0.44
1:G:417:LYS:HD3	1:G:418:LEU:O	2.17	0.44
1:C:269:GLU:O	1:C:269:GLU:HG2	2.16	0.44
1:D:37:ILE:HD13	1:D:37:ILE:N	2.33	0.44
1:E:88:THR:HG22	1:E:194:GLN:HA	1.99	0.44
1:F:424:ILE:HD12	1:F:425:GLN:N	2.32	0.44
1:G:51:THR:HA	1:G:54:LEU:HD23	1.99	0.44
1:G:377:SER:HB2	1:G:382:VAL:CG2	2.48	0.44
1:A:127:ILE:O	1:A:130:GLU:O	2.36	0.44
1:B:172:ILE:HD12	1:B:175:CYS:CB	2.47	0.44
1:D:166:LEU:O	1:D:167:LYS:HB3	2.18	0.44
1:E:299:GLN:NE2	1:E:433:GLN:HG3	2.33	0.44
1:F:37:ILE:HD13	1:F:37:ILE:N	2.33	0.44
1:F:221:PRO:O	1:F:224:ILE:HG23	2.18	0.44
1:G:141:THR:HB	1:G:142:THR:H	1.60	0.44
1:A:8:VAL:HG12	1:A:114:ALA:HB3	2.00	0.44
1:B:48:SER:HA	1:B:51:THR:OG1	2.18	0.44
1:C:371:TRP:CA	1:C:374:THR:HG23	2.45	0.44
1:C:392:GLU:CD	2:C:501:U2F:O6	2.56	0.44
1:E:90:LEU:HD12	1:E:90:LEU:H	1.83	0.44
1:E:123:GLN:HA	1:E:125:LEU:CD1	2.48	0.44
1:E:146:LEU:HD23	1:E:146:LEU:C	2.37	0.44
1:E:304:VAL:HG21	1:E:350:TRP:O	2.17	0.44
1:F:35:ILE:HD12	1:F:35:ILE:N	2.32	0.44
1:F:88:THR:HG22	1:F:194:GLN:HA	2.00	0.44
1:G:80:ILE:HD11	1:G:84:THR:OG1	2.18	0.44
1:G:104:THR:O	1:G:104:THR:OG1	2.25	0.44
1:A:68:ILE:H	1:A:68:ILE:HG13	1.53	0.43
1:B:338:THR:HA	1:B:341:LYS:CD	2.45	0.43
1:D:257:ASP:OD1	1:D:259:VAL:HG23	2.18	0.43
1:F:94:VAL:HG11	1:F:121:CYS:HA	2.00	0.43
1:G:105:ILE:HD13	1:G:105:ILE:HA	1.75	0.43
1:G:180:PRO:O	1:G:183:VAL:HG13	2.18	0.43
1:A:273:PHE:CE2	1:A:353:GLN:HG3	2.51	0.43
1:C:146:LEU:O	1:C:150:ILE:CD1	2.67	0.43
1:E:175:CYS:SG	1:E:223:THR:HG23	2.58	0.43
1:F:90:LEU:O	1:F:94:VAL:HG23	2.18	0.43
1:F:175:CYS:SG	1:F:223:THR:HG23	2.58	0.43
1:G:33:HIS:CE1	1:G:465:ILE:HG21	2.50	0.43
1:G:124:ILE:N	1:G:124:ILE:CD1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:170:LEU:HG	1:G:178:LEU:HB3	2.00	0.43
1:G:187:LEU:N	1:G:187:LEU:HD22	2.32	0.43
1:G:410:PRO:HA	1:G:427:MET:CE	2.48	0.43
1:A:128:ALA:HA	1:A:133:ILE:HD13	2.01	0.43
1:B:136:TYR:CE1	1:B:472:ILE:HD13	2.54	0.43
1:D:20:ILE:HG21	1:D:249:ARG:HG3	1.98	0.43
1:E:35:ILE:HD12	1:E:35:ILE:N	2.33	0.43
1:G:8:VAL:O	1:G:37:ILE:HG12	2.17	0.43
1:G:137:THR:HG23	1:G:208:PHE:CD2	2.52	0.43
1:G:234:ARG:HH11	1:G:238:LYS:HZ3	1.63	0.43
1:G:262:TRP:CG	1:G:345:LEU:HD12	2.53	0.43
1:A:455:LEU:HD12	1:A:455:LEU:N	2.33	0.43
1:A:466:CYS:HA	1:A:469:VAL:HG22	2.00	0.43
1:C:13:SER:CA	1:C:42:ILE:HD11	2.47	0.43
1:C:117:VAL:HG11	1:C:121:CYS:C	2.38	0.43
1:C:332:LEU:HD21	1:C:333:PRO:O	2.18	0.43
1:C:335:GLY:C	1:C:339:ARG:NH1	2.72	0.43
1:D:95:ARG:CA	1:D:98:LEU:HD23	2.48	0.43
1:E:73:SER:HB3	1:E:93:LEU:HD11	2.00	0.43
1:E:166:LEU:CD1	1:E:168:GLU:H	2.31	0.43
1:E:235:LEU:HD13	1:E:235:LEU:O	2.19	0.43
1:E:373:SER:OG	2:E:501:U2F:C5'	2.48	0.43
1:F:235:LEU:O	1:F:235:LEU:HD13	2.18	0.43
2:F:501:U2F:O6'	2:F:501:U2F:O4'	2.35	0.43
1:G:197:GLU:CA	1:G:200:LYS:HG3	2.48	0.43
1:G:292:TRP:C	1:G:296:LEU:HD22	2.38	0.43
1:G:328:MET:HA	1:G:331:TYR:CZ	2.54	0.43
1:A:57:THR:O	1:A:60:THR:HG22	2.18	0.43
1:A:125:LEU:N	1:A:126:PRO:HD2	2.33	0.43
1:A:180:PRO:O	1:A:183:VAL:HG13	2.19	0.43
1:A:370:GLY:HA3	2:A:501:U2F:F1	2.08	0.43
1:A:419:VAL:HG12	1:A:424:ILE:HD11	2.00	0.43
1:B:76:ILE:CD1	1:B:93:LEU:HD22	2.48	0.43
1:C:35:ILE:HD12	1:C:35:ILE:N	2.32	0.43
1:C:164:VAL:HG11	1:C:188:LEU:HA	1.99	0.43
1:D:20:ILE:CG2	1:D:249:ARG:HG3	2.48	0.43
1:E:43:THR:OG1	1:E:72:PRO:HA	2.18	0.43
1:E:44:THR:HG21	1:E:47:SER:HG	1.83	0.43
1:E:111:ARG:HH21	1:E:131:PHE:HD1	1.66	0.43
1:E:112:PRO:HG2	1:E:133:ILE:HD13	2.01	0.43
1:F:476:GLU:N	1:F:477:LEU:HD12	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:ILE:C	1:G:119:ILE:HD13	2.39	0.43
1:G:260:ILE:N	1:G:260:ILE:HD12	2.33	0.43
1:A:195:TYR:O	1:A:199:VAL:HG12	2.19	0.43
1:A:231:GLU:O	1:A:235:LEU:CD1	2.58	0.43
1:A:272:LEU:HD23	1:A:428:VAL:HG22	2.00	0.43
1:C:301:PHE:CZ	1:C:344:GLY:HA3	2.53	0.43
1:D:383:PRO:HB2	1:D:431:LEU:HD11	2.01	0.43
1:E:34:ASN:O	1:E:34:ASN:CG	2.57	0.43
1:G:115:LEU:HD13	1:G:115:LEU:HA	1.78	0.43
1:A:130:GLU:HB2	1:A:131:PHE:CD1	2.53	0.43
1:B:94:VAL:O	1:B:98:LEU:CD2	2.67	0.43
1:B:328:MET:O	1:B:332:LEU:CD2	2.66	0.43
1:C:72:PRO:CD	1:C:100:LYS:HE3	2.48	0.43
1:C:144:TRP:CH2	1:C:176:LYS:HD3	2.54	0.43
1:D:78:HIS:CD2	1:D:79:LEU:CD2	3.01	0.43
1:D:111:ARG:NH1	1:D:131:PHE:HE2	2.16	0.43
1:D:117:VAL:CG1	1:D:121:CYS:O	2.66	0.43
1:E:304:VAL:CG2	1:E:351:ALA:HB3	2.49	0.43
1:F:34:ASN:CG	1:F:34:ASN:O	2.57	0.43
1:F:75:ASP:O	1:F:76:ILE:CG2	2.66	0.43
1:F:92:LEU:HD13	1:F:95:ARG:NH1	2.33	0.43
1:G:115:LEU:HD23	1:G:133:ILE:HG13	2.01	0.43
1:G:125:LEU:CG	1:G:126:PRO:CD	2.92	0.43
1:G:155:PHE:CE1	1:G:170:LEU:O	2.72	0.43
1:G:305:VAL:HG13	1:G:346:VAL:HG13	2.00	0.43
1:A:36:LYS:H	1:A:36:LYS:HG3	1.64	0.43
1:A:42:ILE:C	1:A:42:ILE:HD12	2.39	0.43
1:A:127:ILE:CD1	1:A:127:ILE:N	2.81	0.43
1:A:272:LEU:CD2	1:A:428:VAL:HG22	2.48	0.43
1:B:10:ILE:HA	1:B:116:ILE:O	2.18	0.43
1:C:10:ILE:CG2	1:C:22:VAL:HG23	2.48	0.43
1:C:16:MET:HE1	1:C:49:ALA:CB	2.49	0.43
1:C:109:THR:HG23	1:C:110:HIS:CG	2.53	0.43
1:C:277:GLY:HA3	1:C:368:HIS:CE1	2.54	0.43
1:C:328:MET:CE	1:C:331:TYR:OH	2.67	0.43
1:D:42:ILE:CD1	1:D:94:VAL:HG13	2.49	0.43
1:D:148:LEU:C	1:D:148:LEU:HD13	2.39	0.43
1:D:301:PHE:CZ	1:D:344:GLY:HA3	2.54	0.43
1:D:435:LYS:HB2	1:G:217:GLU:HG2	2.01	0.43
1:E:25:LEU:O	1:E:29:LEU:HD12	2.18	0.43
1:E:155:PHE:CZ	1:E:172:ILE:CD1	3.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:SER:O	1:F:51:THR:N	2.51	0.43
1:F:426:GLY:C	1:F:430:ILE:HD13	2.39	0.43
1:G:383:PRO:HB2	1:G:431:LEU:HD11	2.01	0.43
1:G:461:SER:O	1:G:465:ILE:HD12	2.18	0.43
1:A:433:GLN:HE22	1:A:434:THR:HG22	1.83	0.43
1:C:10:ILE:CG2	1:C:22:VAL:CG2	2.96	0.43
1:E:176:LYS:HE2	1:E:403:GLU:OE1	2.19	0.43
1:E:244:ILE:HG13	1:E:244:ILE:O	2.18	0.43
1:E:292:TRP:C	1:E:296:LEU:HD22	2.39	0.43
1:F:10:ILE:HA	1:F:116:ILE:O	2.19	0.43
1:G:10:ILE:HA	1:G:116:ILE:O	2.18	0.43
1:G:91:ARG:HH21	1:G:95:ARG:NH1	2.17	0.43
1:G:164:VAL:HG11	1:G:188:LEU:HD13	2.00	0.43
1:A:292:TRP:C	1:A:296:LEU:HD12	2.30	0.43
1:C:387:TRP:CH2	1:C:419:VAL:HG21	2.53	0.43
1:E:119:ILE:HD12	1:E:119:ILE:C	2.39	0.43
1:F:95:ARG:CA	1:F:98:LEU:HD23	2.49	0.43
1:F:286:GLN:NE2	1:F:387:TRP:CZ2	2.87	0.43
1:F:293:GLY:CA	1:F:424:ILE:CD1	2.91	0.43
1:F:425:GLN:HA	1:F:428:VAL:CG1	2.49	0.43
1:A:148:LEU:C	1:A:148:LEU:HD13	2.39	0.42
1:A:383:PRO:HB2	1:A:431:LEU:HD11	2.01	0.42
1:C:13:SER:HB3	1:C:118:ASP:OD2	2.19	0.42
1:C:408:ILE:CD1	1:C:430:ILE:HG13	2.50	0.42
1:D:27:ASN:HA	1:D:66:ILE:HD11	2.01	0.42
1:D:117:VAL:HG21	1:D:124:ILE:HB	2.01	0.42
1:D:249:ARG:NH2	2:D:501:U2F:O6'	2.52	0.42
1:D:413:LEU:HD21	1:D:415:THR:HG23	2.00	0.42
1:E:119:ILE:HG21	1:E:140:PRO:HD2	2.00	0.42
1:E:466:CYS:HA	1:E:469:VAL:HG12	2.01	0.42
1:F:352:ASN:OD1	1:F:355:GLU:CG	2.67	0.42
1:G:170:LEU:HD21	1:G:178:LEU:H	1.84	0.42
1:A:48:SER:O	1:A:52:GLU:HG3	2.19	0.42
1:A:49:ALA:O	1:A:52:GLU:CD	2.57	0.42
1:B:27:ASN:OD1	1:B:66:ILE:HD13	2.19	0.42
1:B:43:THR:OG1	1:B:72:PRO:HA	2.19	0.42
1:B:95:ARG:CA	1:B:98:LEU:HD23	2.48	0.42
1:B:377:SER:OG	1:B:384:MET:HE1	2.18	0.42
1:C:335:GLY:HA3	1:C:339:ARG:HH12	1.83	0.42
1:D:370:GLY:HA2	2:D:501:U2F:O4	2.19	0.42
1:E:119:ILE:CG1	1:E:120:PHE:CD1	2.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:GLN:HA	1:E:125:LEU:HD11	2.01	0.42
1:F:268:ASN:HD21	1:G:438:LYS:HD2	1.83	0.42
1:F:301:PHE:CZ	1:F:344:GLY:HA3	2.54	0.42
1:G:410:PRO:CA	1:G:427:MET:CE	2.98	0.42
2:A:501:U2F:C5	3:A:502:T83:OAC	2.67	0.42
1:B:137:THR:HG21	1:B:205:TYR:HD1	1.81	0.42
1:B:431:LEU:O	1:B:432:MET:HB2	2.19	0.42
1:D:400:LEU:HD22	1:D:400:LEU:H	1.83	0.42
1:E:6:LEU:CD1	1:E:473:ARG:HD3	2.46	0.42
1:E:192:ASP:O	1:E:193:GLN:C	2.58	0.42
1:E:469:VAL:HG13	1:E:470:LYS:CE	2.49	0.42
1:F:276:PHE:CD1	1:F:276:PHE:N	2.87	0.42
1:G:53:PHE:CD1	1:G:56:LYS:HE2	2.54	0.42
1:G:88:THR:HG23	1:G:194:GLN:CB	2.44	0.42
1:G:197:GLU:HA	1:G:200:LYS:CG	2.49	0.42
1:G:304:VAL:HG22	1:G:347:VAL:CG2	2.49	0.42
1:A:14:PRO:HA	1:A:42:ILE:O	2.19	0.42
1:A:16:MET:HE3	1:A:16:MET:HB3	1.95	0.42
1:A:465:ILE:HG12	1:A:466:CYS:N	2.33	0.42
1:A:469:VAL:CA	1:A:472:ILE:HG23	2.48	0.42
1:B:237:LEU:HD22	1:B:239:VAL:O	2.18	0.42
1:C:38:THR:CG2	1:C:69:ILE:HG12	2.50	0.42
1:C:147:ALA:O	1:C:150:ILE:HD13	2.20	0.42
1:E:154:VAL:O	1:E:157:LYS:CG	2.67	0.42
1:E:328:MET:HG3	1:E:331:TYR:CE2	2.54	0.42
1:F:12:SER:O	1:F:13:SER:HB3	2.20	0.42
1:F:78:HIS:CE1	1:F:79:LEU:HB2	2.53	0.42
1:F:137:THR:HG21	1:F:205:TYR:HE1	1.84	0.42
1:G:301:PHE:CZ	1:G:344:GLY:HA3	2.54	0.42
1:B:94:VAL:HG11	1:B:121:CYS:HA	2.01	0.42
1:B:272:LEU:HD21	1:B:428:VAL:HG12	2.00	0.42
1:B:301:PHE:CZ	1:B:344:GLY:HA3	2.54	0.42
1:C:69:ILE:HD13	1:C:69:ILE:N	2.34	0.42
1:D:20:ILE:O	1:D:24:VAL:HG23	2.18	0.42
1:D:45:THR:O	1:D:46:SER:C	2.58	0.42
1:E:425:GLN:HA	1:E:428:VAL:CG1	2.49	0.42
1:E:463:ASN:HD22	1:E:463:ASN:HA	1.63	0.42
1:F:98:LEU:HD11	1:F:123:GLN:O	2.19	0.42
1:G:18:HIS:O	1:G:22:VAL:HG22	2.19	0.42
1:G:141:THR:HG22	1:G:371:TRP:CG	2.53	0.42
1:G:165:GLU:CD	1:G:165:GLU:N	2.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:GLY:CA	2:A:501:U2F:F1	2.57	0.42
1:B:98:LEU:HD11	1:B:123:GLN:O	2.20	0.42
1:C:146:LEU:O	1:C:150:ILE:HD13	2.19	0.42
1:C:408:ILE:HD12	1:C:430:ILE:CD1	2.48	0.42
1:D:125:LEU:HB3	1:D:126:PRO:HD3	2.01	0.42
1:G:33:HIS:HB3	1:G:35:ILE:HD11	2.01	0.42
1:G:164:VAL:CG1	1:G:188:LEU:HD13	2.50	0.42
1:A:76:ILE:O	1:A:80:ILE:HG22	2.20	0.42
1:B:276:PHE:CD1	1:B:276:PHE:N	2.87	0.42
1:C:118:ASP:OD1	1:C:121:CYS:SG	2.74	0.42
1:D:218:ASP:OD2	1:D:450:SER:HB2	2.20	0.42
1:E:22:VAL:HG22	1:E:23:LEU:HD12	2.02	0.42
1:E:438:LYS:HD2	1:E:438:LYS:H	1.81	0.42
1:G:25:LEU:C	1:G:25:LEU:CD2	2.85	0.42
1:G:90:LEU:CD1	1:G:120:PHE:HB3	2.48	0.42
1:G:179:ARG:HD3	1:G:180:PRO:HD2	2.00	0.42
1:G:234:ARG:HH11	1:G:238:LYS:HZ2	1.66	0.42
1:G:412:VAL:HG11	1:G:417:LYS:HB3	2.01	0.42
1:G:425:GLN:HA	1:G:428:VAL:CG1	2.49	0.42
1:A:88:THR:HG23	1:A:194:GLN:HB3	2.00	0.42
1:C:297:SER:N	1:C:425:GLN:HG3	2.35	0.42
1:C:298:GLN:HE21	1:D:255:LEU:HD23	1.84	0.42
1:D:119:ILE:C	1:D:119:ILE:HD13	2.40	0.42
1:D:234:ARG:HH11	1:D:238:LYS:CA	2.33	0.42
1:F:262:TRP:CE3	1:F:345:LEU:HD12	2.55	0.42
1:F:327:ASP:O	1:F:330:GLU:HG3	2.20	0.42
1:G:57:THR:C	1:G:59:LEU:N	2.71	0.42
1:G:387:TRP:CZ3	1:G:424:ILE:CD1	3.03	0.42
1:A:126:PRO:O	1:A:130:GLU:HG3	2.19	0.42
1:A:462:TYR:CA	1:A:465:ILE:HD13	2.49	0.42
1:C:72:PRO:CD	1:C:100:LYS:CE	2.98	0.42
1:C:94:VAL:O	1:C:98:LEU:CD1	2.68	0.42
1:C:248:ARG:CG	1:C:375:VAL:HG12	2.49	0.42
1:D:333:PRO:O	1:D:334:GLU:O	2.37	0.42
1:D:353:GLN:OE1	1:D:376:GLU:OE1	2.38	0.42
2:D:501:U2F:O3	3:D:502:T83:CAJ	2.68	0.42
1:E:48:SER:OG	1:E:52:GLU:HG3	2.20	0.42
1:F:27:ASN:HA	1:F:66:ILE:HD11	2.01	0.42
1:F:94:VAL:O	1:F:98:LEU:CD2	2.67	0.42
1:F:148:LEU:HD13	1:F:148:LEU:C	2.40	0.42
1:F:337:LEU:HD22	1:F:337:LEU:N	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:ARG:CZ	1:G:349:MET:O	2.68	0.42
1:G:368:HIS:NE2	2:G:501:U2F:O2B	2.44	0.42
1:G:436:GLU:HG3	1:G:439:ARG:HH21	1.85	0.42
1:A:144:TRP:HA	1:A:223:THR:HG21	2.01	0.42
1:B:155:PHE:HD1	1:B:159:ILE:HD11	1.84	0.42
1:B:425:GLN:HA	1:B:428:VAL:HG22	2.01	0.42
1:C:292:TRP:C	1:C:296:LEU:HD22	2.39	0.42
1:D:52:GLU:HA	1:D:55:LYS:HG2	2.02	0.42
1:D:94:VAL:O	1:D:98:LEU:CD2	2.68	0.42
1:E:137:THR:HG21	1:E:205:TYR:HE1	1.85	0.42
1:F:105:ILE:HA	1:F:108:MET:HE3	2.01	0.42
1:G:40:LEU:HA	1:G:69:ILE:HG23	2.02	0.42
1:G:155:PHE:CZ	1:G:172:ILE:CD1	3.02	0.42
1:C:59:LEU:HD23	1:C:68:ILE:N	2.32	0.41
1:C:137:THR:HG21	1:C:205:TYR:HE1	1.85	0.41
1:E:6:LEU:CD1	1:E:473:ARG:HH11	2.31	0.41
1:E:148:LEU:HD13	1:E:148:LEU:C	2.41	0.41
1:F:10:ILE:HG21	1:F:22:VAL:HG13	2.00	0.41
1:F:92:LEU:CD1	1:F:95:ARG:NH1	2.83	0.41
1:F:125:LEU:CD1	1:F:135:LYS:HD2	2.49	0.41
1:G:166:LEU:CD1	1:G:168:GLU:HB2	2.48	0.41
1:G:466:CYS:HA	1:G:469:VAL:CG1	2.49	0.41
1:A:66:ILE:O	1:A:66:ILE:HG12	2.19	0.41
1:B:106:ALA:HA	1:B:111:ARG:NH1	2.34	0.41
1:B:440:ILE:CD1	1:B:440:ILE:N	2.72	0.41
2:D:501:U2F:O3	2:D:501:U2F:O6	2.35	0.41
1:E:118:ASP:CB	1:E:121:CYS:SG	3.06	0.41
1:E:119:ILE:CG1	1:E:120:PHE:CE1	3.03	0.41
1:E:159:ILE:HG22	1:E:190:ARG:NH2	2.33	0.41
1:G:127:ILE:O	1:G:130:GLU:HG3	2.19	0.41
1:A:74:VAL:HG13	1:A:100:LYS:NZ	2.35	0.41
1:B:88:THR:HG23	1:B:194:GLN:HB3	2.02	0.41
1:B:114:ALA:HB2	1:B:472:ILE:HG23	2.03	0.41
1:B:234:ARG:NH1	1:B:237:LEU:HD22	2.36	0.41
1:C:37:ILE:CD1	1:C:65:THR:O	2.67	0.41
1:C:59:LEU:CG	1:C:68:ILE:O	2.65	0.41
1:C:250:LYS:HD3	1:C:250:LYS:HA	1.69	0.41
1:C:370:GLY:CA	2:C:501:U2F:HE	2.07	0.41
1:E:124:ILE:N	1:E:124:ILE:CD1	2.83	0.41
1:F:353:GLN:NE2	2:F:501:U2F:H2'	2.34	0.41
1:G:163:TYR:OH	1:G:190:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:LYS:O	1:G:236:LEU:HD13	2.19	0.41
1:G:335:GLY:C	1:G:339:ARG:HH12	2.23	0.41
1:G:463:ASN:HA	1:G:466:CYS:SG	2.60	0.41
1:A:5:GLN:HA	1:A:34:ASN:HD21	1.84	0.41
1:A:10:ILE:HG21	1:A:22:VAL:HG13	2.01	0.41
1:C:57:THR:OG1	1:C:60:THR:CB	2.68	0.41
1:C:213:ILE:HD11	1:C:243:PRO:HG3	2.01	0.41
1:D:328:MET:O	1:D:332:LEU:HD23	2.19	0.41
1:E:74:VAL:HG22	1:E:75:ASP:N	2.34	0.41
1:E:157:LYS:C	1:E:159:ILE:HG12	2.40	0.41
1:F:76:ILE:CD1	1:F:79:LEU:HB3	2.50	0.41
1:F:127:ILE:O	1:F:130:GLU:O	2.38	0.41
1:F:184:VAL:O	1:F:188:LEU:CD2	2.68	0.41
1:F:231:GLU:HG2	1:F:232:LYS:N	2.36	0.41
1:F:262:TRP:CG	1:F:345:LEU:HD12	2.54	0.41
1:G:127:ILE:HD13	1:G:127:ILE:C	2.37	0.41
1:G:195:TYR:O	1:G:199:VAL:HG12	2.21	0.41
1:B:172:ILE:CD1	1:B:175:CYS:CB	2.98	0.41
1:B:372:ASN:HA	1:B:375:VAL:HG22	2.02	0.41
1:D:263:LEU:C	1:D:359:HIS:HE1	2.24	0.41
1:E:158:GLU:C	1:E:159:ILE:HG12	2.40	0.41
1:E:220:GLU:O	1:E:224:ILE:CD1	2.66	0.41
1:G:10:ILE:HG22	1:G:22:VAL:CG1	2.49	0.41
1:G:14:PRO:O	1:G:15:GLY:C	2.58	0.41
1:G:114:ALA:O	1:G:115:LEU:HD22	2.19	0.41
1:A:406:VAL:CG2	1:A:444:ALA:CB	2.89	0.41
1:B:146:LEU:O	1:B:150:ILE:CD1	2.68	0.41
1:D:244:ILE:HB	1:D:465:ILE:CD1	2.51	0.41
1:E:78:HIS:CD2	1:E:79:LEU:HD11	2.56	0.41
1:E:301:PHE:CZ	1:E:344:GLY:HA3	2.55	0.41
1:F:380:ASN:C	1:F:448:LYS:HE3	2.41	0.41
1:G:13:SER:HB3	1:G:14:PRO:CD	2.49	0.41
1:G:268:ASN:C	1:G:269:GLU:CG	2.88	0.41
1:A:61:ASN:HB3	1:A:67:GLU:CD	2.40	0.41
1:A:198:TYR:O	1:A:201:LEU:HB3	2.21	0.41
1:A:365:PHE:HE2	1:A:373:SER:HG	1.62	0.41
1:C:114:ALA:CB	1:C:472:ILE:HD12	2.51	0.41
1:C:230:ASN:OD1	1:C:232:LYS:HD3	2.20	0.41
1:F:33:HIS:HE1	1:F:465:ILE:HD13	1.86	0.41
1:G:38:THR:HB	1:G:67:GLU:HG2	2.02	0.41
1:G:125:LEU:HD12	1:G:126:PRO:CD	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:290:LEU:HD22	1:G:303:TRP:CZ2	2.55	0.41
1:A:106:ALA:O	1:A:107:SER:HB3	2.20	0.41
1:A:327:ASP:OD2	1:A:329:SER:OG	2.36	0.41
1:B:471:ASP:O	1:B:475:ARG:HG2	2.20	0.41
1:C:94:VAL:HG23	1:C:95:ARG:N	2.36	0.41
1:C:252:GLU:O	1:C:254:THR:HG23	2.21	0.41
1:D:144:TRP:CH2	1:D:176:LYS:HD3	2.55	0.41
1:E:10:ILE:HA	1:E:116:ILE:O	2.20	0.41
1:E:401:THR:HG21	1:E:409:ARG:HD3	2.03	0.41
1:F:173:PRO:HB3	1:F:232:LYS:CD	2.44	0.41
1:G:25:LEU:HD23	1:G:29:LEU:CD2	2.45	0.41
1:G:91:ARG:HE	1:G:123:GLN:NE2	2.19	0.41
1:G:162:GLU:CD	1:G:162:GLU:N	2.72	0.41
1:G:336:PHE:HA	1:G:339:ARG:CZ	2.47	0.41
1:A:9:ALA:O	1:A:115:LEU:HA	2.21	0.41
1:A:218:ASP:OD2	1:A:450:SER:HB2	2.21	0.41
1:B:136:TYR:CE1	1:B:472:ILE:CD1	3.04	0.41
1:B:198:TYR:O	1:B:201:LEU:HB3	2.19	0.41
1:B:289:GLU:O	1:B:424:ILE:HD11	2.21	0.41
1:B:292:TRP:N	1:B:295:GLU:OE1	2.53	0.41
1:C:16:MET:CE	1:C:49:ALA:CB	2.98	0.41
1:C:146:LEU:HD23	1:C:146:LEU:O	2.21	0.41
1:C:404:LEU:HD13	1:C:404:LEU:N	2.36	0.41
1:D:6:LEU:HA	1:D:6:LEU:HD22	1.75	0.41
1:D:10:ILE:HA	1:D:116:ILE:O	2.20	0.41
1:D:418:LEU:HD13	1:D:419:VAL:N	2.35	0.41
1:E:32:HIS:HB2	1:E:33:HIS:ND1	2.36	0.41
1:F:19:LEU:HD12	1:F:23:LEU:HD12	2.03	0.41
1:F:231:GLU:OE2	1:F:232:LYS:HE3	2.21	0.41
1:F:273:PHE:C	1:F:273:PHE:CD1	2.94	0.41
1:F:430:ILE:HD12	1:F:430:ILE:N	2.36	0.41
1:F:445:LYS:HB2	1:F:445:LYS:HE2	1.93	0.41
1:G:82:SER:O	1:G:83:SER:HB3	2.21	0.41
1:G:153:GLN:NE2	1:G:203:LYS:HE3	2.29	0.41
1:A:80:ILE:HG12	1:A:81:ASN:N	2.36	0.41
1:A:136:TYR:OH	1:A:471:ASP:CG	2.59	0.41
1:B:209:ASP:C	1:B:239:VAL:CG2	2.89	0.41
1:C:88:THR:HG23	1:C:194:GLN:HB3	2.03	0.41
1:D:155:PHE:CD1	1:D:170:LEU:HD12	2.56	0.41
1:D:345:LEU:HD13	1:D:345:LEU:C	2.41	0.41
1:E:187:LEU:HD21	1:E:198:TYR:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:263:LEU:C	1:E:359:HIS:HE1	2.25	0.41
1:E:276:PHE:CD1	1:E:276:PHE:N	2.88	0.41
1:E:296:LEU:N	1:E:296:LEU:CD1	2.84	0.41
1:G:55:LYS:NZ	1:G:56:LYS:HG2	2.35	0.41
1:G:123:GLN:N	1:G:123:GLN:CD	2.74	0.41
1:G:296:LEU:N	1:G:296:LEU:CD1	2.84	0.41
1:A:133:ILE:N	1:A:133:ILE:CD1	2.84	0.40
1:A:301:PHE:CZ	1:A:344:GLY:HA3	2.55	0.40
1:B:182:ASP:O	1:B:395:MET:HG3	2.21	0.40
1:C:119:ILE:O	1:C:122:THR:HG23	2.21	0.40
1:C:218:ASP:OD2	1:C:450:SER:HB2	2.21	0.40
1:C:297:SER:HB2	1:C:428:VAL:HG23	2.03	0.40
1:D:80:ILE:CG2	1:D:92:LEU:HD12	2.51	0.40
1:E:146:LEU:C	1:E:146:LEU:CD2	2.90	0.40
1:E:255:LEU:CD2	1:E:255:LEU:N	2.84	0.40
1:G:105:ILE:HG23	1:G:108:MET:HE1	2.02	0.40
1:G:249:ARG:CZ	2:G:501:U2F:O2'	2.69	0.40
1:G:305:VAL:HG23	1:G:328:MET:CE	2.47	0.40
1:G:387:TRP:O	1:G:389:LEU:HD22	2.21	0.40
1:A:10:ILE:HG22	1:A:22:VAL:HG13	2.04	0.40
1:A:172:ILE:HD13	1:A:172:ILE:N	2.36	0.40
1:B:273:PHE:CD1	1:B:273:PHE:C	2.94	0.40
1:B:393:GLN:NE2	2:B:501:U2F:O6	2.52	0.40
1:B:427:MET:HA	1:B:430:ILE:HG22	2.03	0.40
1:C:16:MET:HE1	1:C:49:ALA:HB1	1.99	0.40
1:C:213:ILE:HD11	1:C:243:PRO:CG	2.51	0.40
1:D:144:TRP:HA	1:D:223:THR:HG21	2.03	0.40
1:D:234:ARG:HH11	1:D:238:LYS:N	2.20	0.40
1:F:76:ILE:HA	1:F:78:HIS:CD2	2.57	0.40
1:F:209:ASP:C	1:F:239:VAL:CG2	2.89	0.40
1:F:290:LEU:HD23	1:F:290:LEU:C	2.41	0.40
1:F:441:LYS:HG2	1:F:445:LYS:HE3	2.03	0.40
1:F:468:LEU:HD23	1:F:468:LEU:C	2.41	0.40
1:A:19:LEU:HD13	1:A:23:LEU:CD1	2.49	0.40
1:A:389:LEU:O	1:A:390:HIS:CD2	2.75	0.40
1:B:115:LEU:HD22	1:B:117:VAL:HG12	2.03	0.40
1:C:352:ASN:CB	1:C:355:GLU:OE1	2.70	0.40
1:D:137:THR:HG21	1:D:205:TYR:HE1	1.87	0.40
1:E:6:LEU:HD23	1:E:472:ILE:HG21	2.04	0.40
1:E:146:LEU:O	1:E:146:LEU:HD23	2.22	0.40
1:F:421:ARG:HA	1:F:424:ILE:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:20:ILE:CG1	1:G:21:PRO:CD	2.93	0.40
1:G:176:LYS:HE3	1:G:403:GLU:HG3	2.03	0.40
1:G:472:ILE:CG2	1:G:475:ARG:NH1	2.83	0.40
1:C:59:LEU:HD21	1:C:68:ILE:N	2.37	0.40
1:C:125:LEU:HD13	1:C:208:PHE:HE1	1.85	0.40
1:C:353:GLN:HG2	2:C:501:U2F:H3	1.86	0.40
1:C:433:GLN:CG	1:D:264:ASP:OD1	2.70	0.40
1:D:382:VAL:HG12	1:D:383:PRO:O	2.22	0.40
1:E:98:LEU:N	1:E:99:PRO:HD2	2.36	0.40
1:G:44:THR:HG23	1:G:45:THR:O	2.21	0.40
1:G:119:ILE:HG12	1:G:201:LEU:HD21	2.04	0.40
1:A:105:ILE:O	1:A:106:ALA:HB2	2.21	0.40
1:A:469:VAL:C	1:A:472:ILE:HG23	2.41	0.40
1:C:10:ILE:HA	1:C:116:ILE:O	2.20	0.40
1:D:13:SER:HB3	1:D:14:PRO:HD2	2.04	0.40
1:D:25:LEU:O	1:D:29:LEU:HD12	2.21	0.40
1:D:430:ILE:HA	1:D:434:THR:HG21	2.03	0.40
1:E:87:PHE:HB2	1:E:194:GLN:HE21	1.82	0.40
1:E:198:TYR:O	1:E:201:LEU:HB3	2.21	0.40
1:E:441:LYS:HB2	1:E:441:LYS:HE3	1.93	0.40
1:F:263:LEU:C	1:F:359:HIS:HE1	2.25	0.40
1:F:404:LEU:HD13	1:F:447:LEU:HD11	2.03	0.40
1:G:98:LEU:N	1:G:99:PRO:HD2	2.37	0.40
1:G:263:LEU:HD11	1:G:356:ILE:HG23	2.03	0.40
1:G:336:PHE:C	1:G:339:ARG:HH12	2.22	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	454/482 (94%)	403 (89%)	38 (8%)	13 (3%)	4 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	456/482 (95%)	408 (90%)	39 (9%)	9 (2%)	7	33
1	C	456/482 (95%)	411 (90%)	33 (7%)	12 (3%)	5	27
1	D	453/482 (94%)	400 (88%)	39 (9%)	14 (3%)	4	24
1	E	453/482 (94%)	408 (90%)	31 (7%)	14 (3%)	4	24
1	F	456/482 (95%)	414 (91%)	35 (8%)	7 (2%)	10	39
1	G	456/482 (95%)	393 (86%)	46 (10%)	17 (4%)	3	19
All	All	3184/3374 (94%)	2837 (89%)	261 (8%)	86 (3%)	5	26

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	64	LYS
1	A	106	ALA
1	A	189	ASP
1	B	64	LYS
1	B	327	ASP
1	C	58	THR
1	C	60	THR
1	C	111	ARG
1	C	123	GLN
1	D	46	SER
1	D	263	LEU
1	D	336	PHE
1	E	159	ILE
1	E	193	GLN
1	E	194	GLN
1	E	327	ASP
1	F	49	ALA
1	F	329	SER
1	G	50	GLU
1	G	61	ASN
1	G	114	ALA
1	G	171	LYS
1	G	193	GLN
1	G	253	THR
1	G	255	LEU
1	G	277	GLY
1	A	49	ALA
1	A	66	ILE

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Mol	Chain	Res	Type
1	A	329	SER
1	B	46	SER
1	B	255	LEU
1	C	47	SER
1	C	49	ALA
1	C	329	SER
1	D	44	THR
1	D	45	THR
1	D	329	SER
1	D	334	GLU
1	E	191	SER
1	E	255	LEU
1	F	47	SER
1	F	76	ILE
1	G	14	PRO
1	G	194	GLN
1	A	46	SER
1	B	49	ALA
1	B	167	LYS
1	C	255	LEU
1	C	420	LYS
1	D	167	LYS
1	D	253	THR
1	D	255	LEU
1	D	326	ARG
1	E	46	SER
1	G	5	GLN
1	G	167	LYS
1	G	330	GLU
1	A	256	ASN
1	B	47	SER
1	B	328	MET
1	C	124	ILE
1	D	49	ALA
1	E	49	ALA
1	E	253	THR
1	E	328	MET
1	F	48	SER
1	F	254	THR
1	G	256	ASN
1	G	278	SER
1	G	456	SER

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Mol	Chain	Res	Type
1	A	61	ASN
1	B	346	VAL
1	C	421	ARG
1	E	47	SER
1	E	256	ASN
1	E	277	GLY
1	E	351	ALA
1	A	107	SER
1	C	46	SER
1	D	166	LEU
1	A	105	ILE
1	D	277	GLY
1	F	277	GLY
1	G	15	GLY
1	A	277	GLY

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	411/428 (96%)	353 (86%)	58 (14%)	3 15
1	B	413/428 (96%)	372 (90%)	41 (10%)	8 28
1	C	413/428 (96%)	362 (88%)	51 (12%)	4 20
1	D	412/428 (96%)	361 (88%)	51 (12%)	4 19
1	E	412/428 (96%)	355 (86%)	57 (14%)	3 16
1	F	413/428 (96%)	357 (86%)	56 (14%)	3 16
1	G	413/428 (96%)	328 (79%)	85 (21%)	1 4
All	All	2887/2996 (96%)	2488 (86%)	399 (14%)	3 16

All (399) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	13	SER

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Mol	Chain	Res	Type
1	A	16	MET
1	A	24	VAL
1	A	35	ILE
1	A	36	LYS
1	A	42	ILE
1	A	44	THR
1	A	47	SER
1	A	50	GLU
1	A	52	GLU
1	A	54	LEU
1	A	55	LYS
1	A	58	THR
1	A	65	THR
1	A	66	ILE
1	A	68	ILE
1	A	74	VAL
1	A	75	ASP
1	A	76	ILE
1	A	80	ILE
1	A	93	LEU
1	A	98	LEU
1	A	101	ILE
1	A	104	THR
1	A	122	THR
1	A	127	ILE
1	A	131	PHE
1	A	133	ILE
1	A	138	TYR
1	A	159	ILE
1	A	160	GLU
1	A	172	ILE
1	A	175	CYS
1	A	199	VAL
1	A	205	TYR
1	A	235	LEU
1	A	237	LEU
1	A	239	VAL
1	A	247	LEU
1	A	255	LEU
1	A	258	GLU
1	A	259	VAL
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	297	SER
1	A	326	ARG
1	A	331	TYR
1	A	333	PRO
1	A	345	LEU
1	A	352	ASN
1	A	360	SER
1	A	365	PHE
1	A	400	LEU
1	A	425	GLN
1	A	433	GLN
1	A	434	THR
1	A	465	ILE
1	A	472	ILE
1	B	6	LEU
1	B	19	LEU
1	B	37	ILE
1	B	44	THR
1	B	47	SER
1	B	56	LYS
1	B	66	ILE
1	B	74	VAL
1	B	100	LYS
1	B	101	ILE
1	B	104	THR
1	B	105	ILE
1	B	108	MET
1	B	132	ASN
1	B	134	SER
1	B	135	LYS
1	B	138	TYR
1	B	150	ILE
1	B	172	ILE
1	B	175	CYS
1	B	179	ARG
1	B	192	ASP
1	B	205	TYR
1	B	213	ILE
1	B	234	ARG
1	B	235	LEU
1	B	244	ILE
1	B	259	VAL

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Mol	Chain	Res	Type
1	B	273	PHE
1	B	331	TYR
1	B	365	PHE
1	B	375	VAL
1	B	377	SER
1	B	400	LEU
1	B	424	ILE
1	B	438	LYS
1	B	439	ARG
1	B	440	ILE
1	B	461	SER
1	B	465	ILE
1	B	470	LYS
1	C	6	LEU
1	C	13	SER
1	C	16	MET
1	C	37	ILE
1	C	40	LEU
1	C	42	ILE
1	C	45	THR
1	C	47	SER
1	C	53	PHE
1	C	66	ILE
1	C	83	SER
1	C	100	LYS
1	C	102	HIS
1	C	104	THR
1	C	113	ASP
1	C	117	VAL
1	C	124	ILE
1	C	132	ASN
1	C	138	TYR
1	C	148	LEU
1	C	150	ILE
1	C	159	ILE
1	C	160	GLU
1	C	172	ILE
1	C	175	CYS
1	C	178	LEU
1	C	205	TYR
1	C	213	ILE
1	C	231	GLU

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Mol	Chain	Res	Type
1	C	232	LYS
1	C	237	LEU
1	C	239	VAL
1	C	244	ILE
1	C	248	ARG
1	C	249	ARG
1	C	252	GLU
1	C	256	ASN
1	C	259	VAL
1	C	294	LEU
1	C	296	LEU
1	C	328	MET
1	C	331	TYR
1	C	332	LEU
1	C	352	ASN
1	C	361	SER
1	C	374	THR
1	C	392	GLU
1	C	400	LEU
1	C	401	THR
1	C	404	LEU
1	C	476	GLU
1	D	6	LEU
1	D	19	LEU
1	D	22	VAL
1	D	24	VAL
1	D	40	LEU
1	D	55	LYS
1	D	58	THR
1	D	73	SER
1	D	80	ILE
1	D	95	ARG
1	D	104	THR
1	D	105	ILE
1	D	119	ILE
1	D	124	ILE
1	D	133	ILE
1	D	134	SER
1	D	135	LYS
1	D	138	TYR
1	D	157	LYS
1	D	166	LEU

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Mol	Chain	Res	Type
1	D	175	CYS
1	D	179	ARG
1	D	184	VAL
1	D	200	LYS
1	D	205	TYR
1	D	213	ILE
1	D	233	LEU
1	D	235	LEU
1	D	237	LEU
1	D	239	VAL
1	D	247	LEU
1	D	258	GLU
1	D	273	PHE
1	D	297	SER
1	D	326	ARG
1	D	328	MET
1	D	332	LEU
1	D	337	LEU
1	D	361	SER
1	D	365	PHE
1	D	367	THR
1	D	387	TRP
1	D	409	ARG
1	D	412	VAL
1	D	413	LEU
1	D	418	LEU
1	D	456	SER
1	D	465	ILE
1	D	468	LEU
1	D	470	LYS
1	D	477	LEU
1	E	22	VAL
1	E	44	THR
1	E	62	GLU
1	E	74	VAL
1	E	78	HIS
1	E	80	ILE
1	E	81	ASN
1	E	93	LEU
1	E	100	LYS
1	E	104	THR
1	E	108	MET

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Mol	Chain	Res	Type
1	E	119	ILE
1	E	121	CYS
1	E	124	ILE
1	E	125	LEU
1	E	134	SER
1	E	138	TYR
1	E	150	ILE
1	E	154	VAL
1	E	164	VAL
1	E	166	LEU
1	E	168	GLU
1	E	170	LEU
1	E	175	CYS
1	E	183	VAL
1	E	187	LEU
1	E	205	TYR
1	E	219	LEU
1	E	222	GLU
1	E	234	ARG
1	E	237	LEU
1	E	248	ARG
1	E	249	ARG
1	E	250	LYS
1	E	254	THR
1	E	255	LEU
1	E	271	VAL
1	E	273	PHE
1	E	281	THR
1	E	296	LEU
1	E	328	MET
1	E	329	SER
1	E	331	TYR
1	E	332	LEU
1	E	334	GLU
1	E	345	LEU
1	E	361	SER
1	E	365	PHE
1	E	413	LEU
1	E	415	THR
1	E	428	VAL
1	E	431	LEU
1	E	434	THR

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Mol	Chain	Res	Type
1	E	438	LYS
1	E	465	ILE
1	E	470	LYS
1	E	476	GLU
1	F	13	SER
1	F	19	LEU
1	F	23	LEU
1	F	24	VAL
1	F	40	LEU
1	F	43	THR
1	F	59	LEU
1	F	64	LYS
1	F	74	VAL
1	F	76	ILE
1	F	79	LEU
1	F	84	THR
1	F	92	LEU
1	F	93	LEU
1	F	101	ILE
1	F	104	THR
1	F	107	SER
1	F	124	ILE
1	F	129	GLU
1	F	133	ILE
1	F	134	SER
1	F	135	LYS
1	F	138	TYR
1	F	167	LYS
1	F	172	ILE
1	F	175	CYS
1	F	188	LEU
1	F	205	TYR
1	F	219	LEU
1	F	222	GLU
1	F	224	ILE
1	F	232	LYS
1	F	234	ARG
1	F	237	LEU
1	F	244	ILE
1	F	249	ARG
1	F	251	VAL
1	F	273	PHE

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Mol	Chain	Res	Type
1	F	290	LEU
1	F	296	LEU
1	F	329	SER
1	F	331	TYR
1	F	332	LEU
1	F	361	SER
1	F	413	LEU
1	F	418	LEU
1	F	424	ILE
1	F	428	VAL
1	F	433	GLN
1	F	434	THR
1	F	445	LYS
1	F	455	LEU
1	F	456	SER
1	F	457	ASP
1	F	461	SER
1	F	472	ILE
1	G	6	LEU
1	G	18	HIS
1	G	22	VAL
1	G	35	ILE
1	G	36	LYS
1	G	37	ILE
1	G	39	ILE
1	G	40	LEU
1	G	42	ILE
1	G	44	THR
1	G	45	THR
1	G	52	GLU
1	G	54	LEU
1	G	55	LYS
1	G	59	LEU
1	G	67	GLU
1	G	68	ILE
1	G	69	ILE
1	G	76	ILE
1	G	79	LEU
1	G	85	LYS
1	G	86	ILE
1	G	88	THR
1	G	90	LEU

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Mol	Chain	Res	Type
1	G	91	ARG
1	G	92	LEU
1	G	94	VAL
1	G	95	ARG
1	G	101	ILE
1	G	102	HIS
1	G	105	ILE
1	G	108	MET
1	G	115	LEU
1	G	118	ASP
1	G	119	ILE
1	G	124	ILE
1	G	127	ILE
1	G	130	GLU
1	G	133	ILE
1	G	138	TYR
1	G	141	THR
1	G	146	LEU
1	G	148	LEU
1	G	153	GLN
1	G	154	VAL
1	G	162	GLU
1	G	165	GLU
1	G	166	LEU
1	G	170	LEU
1	G	171	LYS
1	G	175	CYS
1	G	187	LEU
1	G	190	ARG
1	G	194	GLN
1	G	197	GLU
1	G	199	VAL
1	G	200	LYS
1	G	213	ILE
1	G	235	LEU
1	G	237	LEU
1	G	239	VAL
1	G	244	ILE
1	G	255	LEU
1	G	259	VAL
1	G	272	LEU
1	G	285	LYS

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Mol	Chain	Res	Type
1	G	294	LEU
1	G	296	LEU
1	G	298	GLN
1	G	326	ARG
1	G	331	TYR
1	G	339	ARG
1	G	365	PHE
1	G	366	LEU
1	G	367	THR
1	G	389	LEU
1	G	394	LYS
1	G	400	LEU
1	G	425	GLN
1	G	428	VAL
1	G	460	SER
1	G	469	VAL
1	G	472	ILE
1	G	475	ARG
1	G	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	61	ASN
1	A	123	GLN
1	A	139	HIS
1	A	193	GLN
1	A	225	ASN
1	A	390	HIS
1	A	433	GLN
1	B	153	GLN
1	B	353	GLN
1	B	393	GLN
1	C	33	HIS
1	C	61	ASN
1	C	78	HIS
1	C	256	ASN
1	C	268	ASN
1	C	298	GLN
1	C	353	GLN
1	C	393	GLN

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Mol	Chain	Res	Type
1	C	433	GLN
1	D	110	HIS
1	D	123	GLN
1	D	225	ASN
1	D	261	GLN
1	D	352	ASN
1	D	353	GLN
1	D	396	ASN
1	D	463	ASN
1	E	78	HIS
1	E	123	GLN
1	E	132	ASN
1	E	153	GLN
1	E	298	GLN
1	E	299	GLN
1	E	352	ASN
1	E	463	ASN
1	F	7	HIS
1	F	61	ASN
1	F	123	GLN
1	F	225	ASN
1	F	261	GLN
1	F	268	ASN
1	F	286	GLN
1	F	425	GLN
1	F	433	GLN
1	G	5	GLN
1	G	7	HIS
1	G	61	ASN
1	G	102	HIS
1	G	123	GLN
1	G	153	GLN
1	G	298	GLN
1	G	359	HIS
1	G	372	ASN
1	G	425	GLN
1	G	433	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	U2F	D	501	-	35,38,38	0.87	1 (2%)	51,58,58	1.47	7 (13%)
2	U2F	G	501	-	35,38,38	0.69	0	51,58,58	1.22	5 (9%)
3	T83	C	502	-	15,15,15	5.85	9 (60%)	21,21,21	4.35	12 (57%)
2	U2F	E	501	-	35,38,38	0.89	2 (5%)	51,58,58	1.98	7 (13%)
3	T83	A	502	-	15,15,15	5.62	9 (60%)	21,21,21	4.61	18 (85%)
2	U2F	B	501	-	35,38,38	0.69	0	51,58,58	1.13	3 (5%)
3	T83	B	502	-	15,15,15	5.70	9 (60%)	21,21,21	4.01	14 (66%)
2	U2F	C	501	-	35,38,38	0.63	0	51,58,58	1.36	8 (15%)
2	U2F	F	501	-	35,38,38	0.84	2 (5%)	51,58,58	1.54	8 (15%)
2	U2F	A	501	-	35,38,38	0.63	1 (2%)	51,58,58	1.17	5 (9%)
3	T83	D	502	-	15,15,15	5.64	9 (60%)	21,21,21	4.25	14 (66%)
3	T83	F	502	-	15,15,15	5.55	9 (60%)	21,21,21	4.89	16 (76%)

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	U2F	D	501	-	-	9/22/59/59	0/3/3/3
2	U2F	G	501	-	-	10/22/59/59	0/3/3/3
3	T83	C	502	-	-	2/2/2/2	0/2/2/2
2	U2F	E	501	-	-	13/22/59/59	0/3/3/3
3	T83	A	502	-	-	2/2/2/2	0/2/2/2
2	U2F	B	501	-	-	6/22/59/59	0/3/3/3
3	T83	B	502	-	-	1/2/2/2	0/2/2/2
2	U2F	C	501	-	-	10/22/59/59	0/3/3/3
2	U2F	F	501	-	-	7/22/59/59	0/3/3/3
2	U2F	A	501	-	-	7/22/59/59	0/3/3/3
3	T83	D	502	-	-	2/2/2/2	0/2/2/2
3	T83	F	502	-	-	2/2/2/2	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	T83	CAF-CAN	14.14	1.64	1.38
3	A	502	T83	CAF-CAN	14.02	1.64	1.38
3	D	502	T83	CAF-CAN	13.58	1.63	1.38
3	F	502	T83	CAF-CAN	13.11	1.62	1.38
3	B	502	T83	CAF-CAN	12.94	1.62	1.38
3	C	502	T83	CAD-CAE	9.75	1.51	1.34
3	B	502	T83	OAI-CAN	-8.54	1.25	1.38
3	B	502	T83	CAD-CAE	8.46	1.49	1.34
3	D	502	T83	CAD-CAE	8.30	1.48	1.34
3	F	502	T83	CAD-CAE	8.28	1.48	1.34
3	A	502	T83	CAD-CAE	8.27	1.48	1.34
3	F	502	T83	OAI-CAN	-8.27	1.25	1.38
3	A	502	T83	OAI-CAN	-7.71	1.26	1.38
3	D	502	T83	OAI-CAN	-7.44	1.27	1.38
3	B	502	T83	CAJ-CAK	-7.41	1.26	1.40
3	C	502	T83	CAJ-CAK	-7.26	1.27	1.40
3	D	502	T83	CAJ-CAK	-7.11	1.27	1.40
3	F	502	T83	CAJ-CAK	-6.98	1.27	1.40
3	F	502	T83	CAG-CAK	-6.61	1.26	1.38
3	C	502	T83	OAI-CAN	-6.54	1.28	1.38
3	A	502	T83	CAG-CAK	-5.85	1.28	1.38
3	C	502	T83	CAG-CAK	-5.85	1.28	1.38
3	B	502	T83	CAG-CAK	-5.76	1.28	1.38
3	D	502	T83	OAC-CAJ	5.72	1.48	1.36
3	B	502	T83	OAH-CAK	5.66	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	502	T83	CAG-CAK	-5.64	1.28	1.38
3	A	502	T83	OAC-CAJ	5.58	1.47	1.36
3	C	502	T83	OAH-CAK	5.48	1.45	1.37
3	A	502	T83	CAJ-CAK	-5.41	1.30	1.40
3	D	502	T83	OAH-CAK	5.34	1.45	1.37
3	C	502	T83	OAC-CAJ	5.24	1.47	1.36
3	A	502	T83	OAH-CAK	4.98	1.45	1.37
3	B	502	T83	OAC-CAJ	4.94	1.46	1.36
3	A	502	T83	CAM-CAN	4.74	1.50	1.41
3	F	502	T83	OAC-CAJ	4.70	1.46	1.36
3	F	502	T83	CAM-CAN	4.63	1.50	1.41
3	C	502	T83	CAM-CAN	4.27	1.49	1.41
3	B	502	T83	CAM-CAN	4.24	1.49	1.41
3	D	502	T83	CAM-CAN	4.04	1.49	1.41
3	B	502	T83	CAD-CAL	3.26	1.52	1.44
2	F	501	U2F	C4-C5	2.89	1.59	1.53
3	F	502	T83	OAH-CAK	2.87	1.41	1.37
2	D	501	U2F	O5-C5	2.77	1.51	1.44
3	C	502	T83	CAD-CAL	2.74	1.50	1.44
2	E	501	U2F	O5-C5	2.60	1.50	1.44
3	F	502	T83	CAD-CAL	2.51	1.50	1.44
2	E	501	U2F	C4-C5	2.48	1.58	1.53
2	A	501	U2F	C4-C5	2.32	1.57	1.53
3	A	502	T83	CAD-CAL	2.27	1.49	1.44
2	F	501	U2F	PB-O1	2.11	1.66	1.60
3	D	502	T83	CAD-CAL	2.10	1.49	1.44

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	T83	OAI-CAN-CAM	9.90	132.68	120.55
3	C	502	T83	OAI-CAN-CAM	9.50	132.18	120.55
3	F	502	T83	CAG-CAK-CAJ	9.22	130.00	120.06
3	D	502	T83	OAI-CAN-CAM	9.17	131.78	120.55
3	B	502	T83	OAI-CAN-CAM	8.96	131.52	120.55
3	A	502	T83	OAI-CAN-CAM	8.95	131.51	120.55
3	B	502	T83	CAF-CAJ-CAK	7.44	127.43	119.81
3	C	502	T83	CAG-CAM-CAN	7.38	128.21	119.40
3	A	502	T83	OAH-CAK-CAG	-7.37	111.44	124.12
3	F	502	T83	OAH-CAK-CAG	-7.37	111.44	124.12
2	E	501	U2F	O5-C1-O1	7.36	120.99	111.36
3	B	502	T83	CAG-CAK-CAJ	7.16	127.77	120.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	502	T83	CAG-CAM-CAN	7.08	127.86	119.40
3	C	502	T83	CAF-CAN-CAM	-6.96	105.57	120.07
3	D	502	T83	CAG-CAM-CAN	6.80	127.52	119.40
3	F	502	T83	CAF-CAJ-CAK	6.79	126.76	119.81
2	F	501	U2F	O5-C1-O1	-6.74	102.56	111.36
3	A	502	T83	CAG-CAM-CAN	6.68	127.38	119.40
3	A	502	T83	CAG-CAK-CAJ	6.60	127.17	120.06
3	D	502	T83	CAF-CAN-CAM	-6.42	106.69	120.07
3	C	502	T83	CAF-CAJ-CAK	6.20	126.15	119.81
3	A	502	T83	CAF-CAN-CAM	-6.16	107.24	120.07
3	D	502	T83	CAG-CAK-CAJ	6.14	126.67	120.06
3	C	502	T83	OAI-CAL-OAB	6.04	124.14	116.44
3	D	502	T83	OAI-CAL-OAB	5.94	124.01	116.44
3	D	502	T83	CAF-CAJ-CAK	5.64	125.58	119.81
3	B	502	T83	CAG-CAM-CAN	5.60	126.08	119.40
3	C	502	T83	CAG-CAK-CAJ	5.44	125.92	120.06
3	F	502	T83	CAF-CAN-CAM	-5.43	108.77	120.07
2	E	501	U2F	C2'-C3'-C4'	-5.41	92.13	102.64
2	E	501	U2F	F1-C2-C3	5.39	113.64	108.85
3	C	502	T83	CAN-CAM-CAE	-5.26	110.66	117.86
3	A	502	T83	CAF-CAJ-CAK	5.23	125.16	119.81
3	D	502	T83	OAH-CAK-CAG	-4.99	115.54	124.12
3	A	502	T83	OAB-CAL-CAD	-4.97	116.76	126.00
3	B	502	T83	CAF-CAN-CAM	-4.90	109.86	120.07
3	A	502	T83	OAI-CAL-OAB	4.82	122.58	116.44
3	A	502	T83	OAH-CAK-CAJ	4.71	121.39	114.57
2	A	501	U2F	PA-O3A-PB	-4.71	116.68	132.83
3	C	502	T83	OAH-CAK-CAG	-4.69	116.05	124.12
2	B	501	U2F	PA-O3A-PB	-4.69	116.74	132.83
3	F	502	T83	OAI-CAL-OAB	4.59	122.29	116.44
3	F	502	T83	CAM-CAG-CAK	-4.48	113.43	120.73
3	B	502	T83	CAJ-CAF-CAN	-4.34	112.97	119.14
3	D	502	T83	OAB-CAL-CAD	-4.33	117.95	126.00
2	E	501	U2F	PA-O3A-PB	-4.31	118.05	132.83
3	C	502	T83	OAI-CAN-CAF	4.30	122.25	115.79
2	E	501	U2F	C1-C2-C3	-4.25	104.35	110.60
3	A	502	T83	CAA-OAH-CAK	-4.24	111.13	117.53
3	F	502	T83	CAJ-CAF-CAN	-4.19	113.17	119.14
3	D	502	T83	CAN-CAM-CAE	-4.17	112.16	117.86
2	D	501	U2F	C1-C2-C3	4.04	116.55	110.60
2	G	501	U2F	PA-O3A-PB	-4.03	119.01	132.83
3	F	502	T83	CAN-CAM-CAE	-4.01	112.37	117.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	U2F	PB-O1-C1	4.00	135.19	119.74
3	D	502	T83	OAI-CAN-CAF	3.83	121.53	115.79
2	D	501	U2F	C1-O5-C5	3.80	121.15	113.69
3	F	502	T83	CAA-OAH-CAK	-3.77	111.84	117.53
3	B	502	T83	OAH-CAK-CAG	-3.67	117.81	124.12
3	A	502	T83	OAI-CAN-CAF	3.64	121.25	115.79
2	G	501	U2F	C1-C2-C3	3.62	115.93	110.60
2	B	501	U2F	F1-C2-C1	3.62	111.62	107.57
2	F	501	U2F	F1-C2-C1	3.59	111.59	107.57
3	F	502	T83	OAB-CAL-CAD	-3.59	119.33	126.00
3	A	502	T83	CAN-CAM-CAE	-3.57	112.97	117.86
2	D	501	U2F	PA-O3A-PB	-3.54	120.69	132.83
3	C	502	T83	OAB-CAL-CAD	-3.41	119.67	126.00
2	C	501	U2F	O2'-C2'-C3'	-3.32	101.07	111.82
3	A	502	T83	CAN-OAI-CAL	-3.31	117.27	121.65
2	D	501	U2F	O5-C5-C4	3.22	115.54	109.69
2	F	501	U2F	O3A-PB-O1	3.16	108.85	102.48
2	F	501	U2F	O1-C1-C2	3.08	114.02	108.38
3	B	502	T83	CAN-CAM-CAE	-3.07	113.67	117.86
3	B	502	T83	CAM-CAG-CAK	-2.97	115.89	120.73
2	F	501	U2F	O3'-C3'-C2'	2.96	121.40	111.82
3	F	502	T83	CAN-OAI-CAL	-2.91	117.80	121.65
2	D	501	U2F	F1-C2-C1	2.89	110.81	107.57
3	B	502	T83	CAN-OAI-CAL	-2.86	117.86	121.65
2	E	501	U2F	F1-C2-C1	2.80	110.70	107.57
3	F	502	T83	OAH-CAK-CAJ	2.74	118.54	114.57
3	B	502	T83	OAB-CAL-CAD	-2.74	120.91	126.00
2	G	501	U2F	O3A-PB-O1	-2.73	96.99	102.48
2	C	501	U2F	O3A-PB-O1	2.71	107.94	102.48
2	F	501	U2F	C6-C5-C4	2.65	119.21	113.00
3	F	502	T83	CAM-CAE-CAD	-2.63	117.93	121.54
2	C	501	U2F	O2'-C2'-C1'	2.61	118.75	110.02
3	A	502	T83	OAC-CAJ-CAF	-2.61	112.48	119.46
2	D	501	U2F	O1-PB-O1B	2.60	119.21	109.47
3	F	502	T83	OAC-CAJ-CAF	-2.59	112.51	119.46
2	A	501	U2F	F1-C2-C1	2.59	110.47	107.57
2	G	501	U2F	C3-C4-C5	2.59	114.86	110.24
2	C	501	U2F	O4-C4-C3	2.45	116.00	110.35
3	B	502	T83	CAM-CAE-CAD	-2.41	118.23	121.54
3	B	502	T83	CAE-CAD-CAL	-2.40	118.33	121.43
2	C	501	U2F	F1-C2-C1	2.39	110.24	107.57
3	A	502	T83	CAM-CAG-CAK	-2.38	116.85	120.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	T83	OAH-CAK-CAJ	2.38	118.01	114.57
3	A	502	T83	OAI-CAL-CAD	2.32	120.66	117.12
3	D	502	T83	CAM-CAG-CAK	-2.29	117.00	120.73
2	C	501	U2F	PA-O3A-PB	-2.28	125.00	132.83
2	D	501	U2F	F1-C2-C3	-2.22	106.88	108.85
3	D	502	T83	OAH-CAK-CAJ	2.22	117.79	114.57
3	A	502	T83	CAM-CAE-CAD	-2.22	118.49	121.54
2	A	501	U2F	O2A-PA-O1A	2.19	123.09	112.24
3	D	502	T83	CAN-OAI-CAL	-2.18	118.76	121.65
2	B	501	U2F	F1-C2-C3	2.18	110.78	108.85
3	B	502	T83	OAI-CAL-CAD	2.15	120.39	117.12
2	C	501	U2F	O5-C1-O1	2.15	114.17	111.36
2	F	501	U2F	O2B-PB-O1B	2.13	122.76	112.24
2	F	501	U2F	C1-O5-C5	2.12	117.84	113.69
2	E	501	U2F	O3'-C3'-C4'	2.10	117.11	111.05
2	A	501	U2F	O2B-PB-O1B	2.09	122.58	112.24
3	D	502	T83	CAM-CAE-CAD	-2.08	118.69	121.54
3	A	502	T83	CAJ-CAF-CAN	-2.08	116.19	119.14
2	G	501	U2F	O2'-C2'-C1'	2.06	116.92	110.02
3	C	502	T83	CAM-CAG-CAK	-2.02	117.45	120.73
2	A	501	U2F	O3A-PB-O1	2.00	106.53	102.48

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	U2F	O5-C1-O1-PB
2	A	501	U2F	PB-O3A-PA-O5'
2	B	501	U2F	PA-O3A-PB-O1
2	C	501	U2F	C5'-O5'-PA-O3A
2	C	501	U2F	C4'-C5'-O5'-PA
2	D	501	U2F	O5-C1-O1-PB
2	D	501	U2F	PB-O3A-PA-O5'
2	D	501	U2F	C3'-C4'-C5'-O5'
2	E	501	U2F	O5-C1-O1-PB
2	E	501	U2F	C5'-O5'-PA-O1A
2	E	501	U2F	C4'-C5'-O5'-PA
2	E	501	U2F	O4'-C4'-C5'-O5'
2	E	501	U2F	C3'-C4'-C5'-O5'
2	F	501	U2F	O5-C1-O1-PB
2	F	501	U2F	O4'-C4'-C5'-O5'
2	F	501	U2F	O4'-C1'-N1-C6'

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Mol	Chain	Res	Type	Atoms
2	F	501	U2F	O4'-C1'-N1-C9'
2	G	501	U2F	O5-C1-O1-PB
2	G	501	U2F	C5'-O5'-PA-O3A
2	C	501	U2F	C4-C5-C6-O6
3	D	502	T83	CAJ-CAK-OAH-CAA
2	A	501	U2F	C4-C5-C6-O6
3	A	502	T83	CAG-CAK-OAH-CAA
2	C	501	U2F	O4'-C4'-C5'-O5'
2	F	501	U2F	C3'-C4'-C5'-O5'
3	D	502	T83	CAG-CAK-OAH-CAA
2	C	501	U2F	O5-C5-C6-O6
3	A	502	T83	CAJ-CAK-OAH-CAA
2	G	501	U2F	O5-C5-C6-O6
3	C	502	T83	CAG-CAK-OAH-CAA
2	A	501	U2F	O5-C5-C6-O6
2	C	501	U2F	C3'-C4'-C5'-O5'
2	D	501	U2F	O4'-C4'-C5'-O5'
2	G	501	U2F	O4'-C4'-C5'-O5'
2	G	501	U2F	C3'-C4'-C5'-O5'
3	F	502	T83	CAG-CAK-OAH-CAA
2	G	501	U2F	C4-C5-C6-O6
2	B	501	U2F	O5-C5-C6-O6
3	C	502	T83	CAJ-CAK-OAH-CAA
2	E	501	U2F	C2'-C1'-N1-C6'
2	A	501	U2F	C1-O1-PB-O3A
3	F	502	T83	CAJ-CAK-OAH-CAA
2	E	501	U2F	C2'-C1'-N1-C9'
2	B	501	U2F	C4-C5-C6-O6
2	C	501	U2F	PA-O3A-PB-O1B
2	B	501	U2F	C4'-C5'-O5'-PA
2	G	501	U2F	C4'-C5'-O5'-PA
2	E	501	U2F	PA-O3A-PB-O1
2	E	501	U2F	PB-O3A-PA-O5'
2	F	501	U2F	PA-O3A-PB-O1
2	G	501	U2F	PA-O3A-PB-O1
2	E	501	U2F	O4'-C1'-N1-C9'
2	E	501	U2F	C5'-O5'-PA-O3A
2	B	501	U2F	PB-O3A-PA-O1A
2	D	501	U2F	C4'-C5'-O5'-PA
2	C	501	U2F	C5'-O5'-PA-O1A
2	E	501	U2F	C5'-O5'-PA-O2A
2	G	501	U2F	C5'-O5'-PA-O1A

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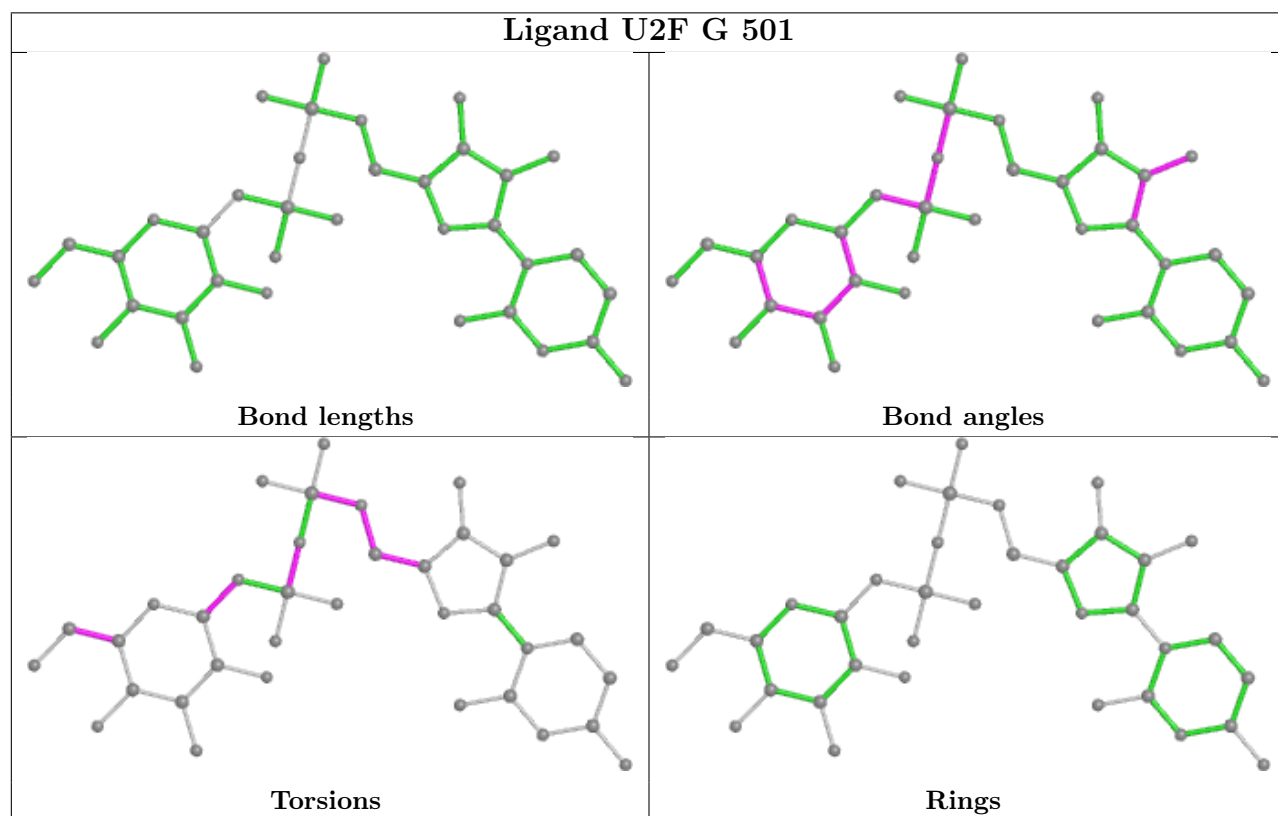
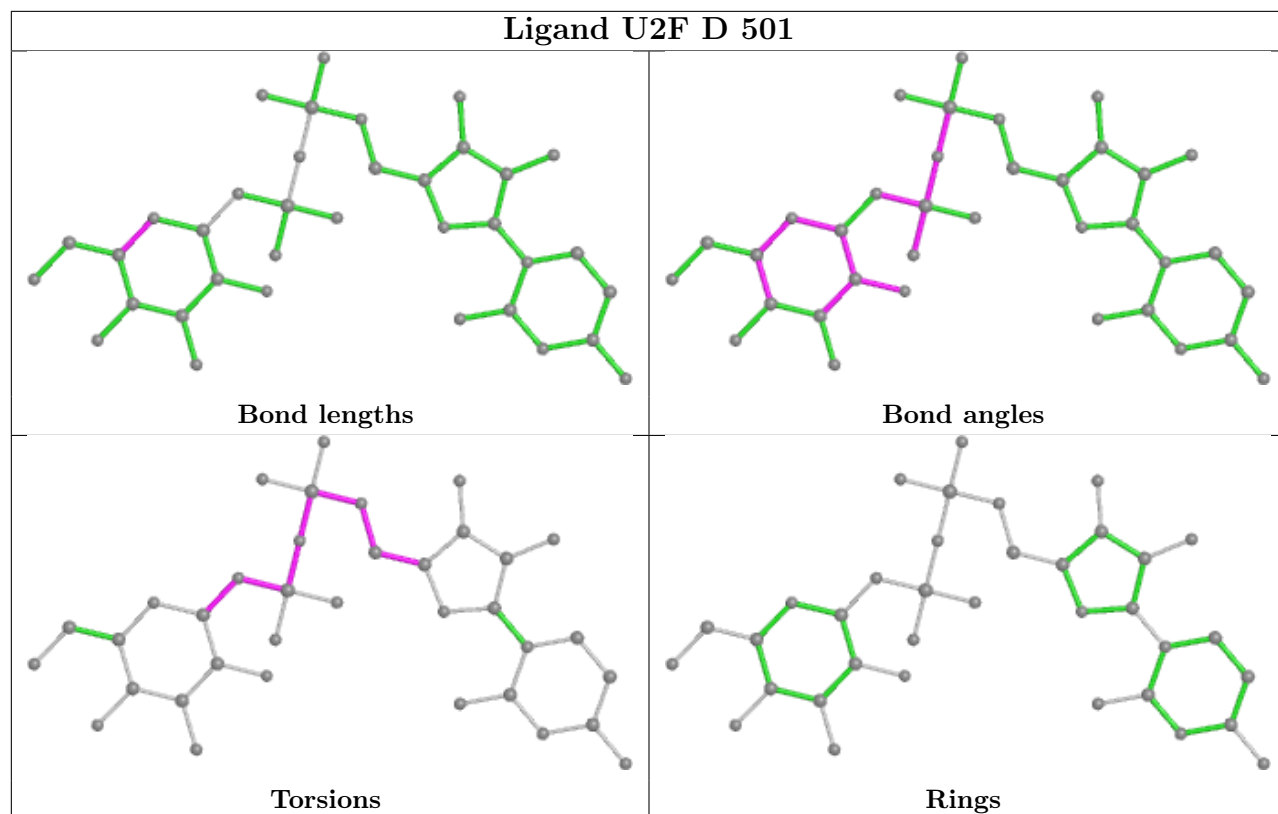
Mol	Chain	Res	Type	Atoms
2	G	501	U2F	C5'-O5'-PA-O2A
2	E	501	U2F	O4'-C1'-N1-C6'
2	F	501	U2F	PA-O3A-PB-O1B
2	D	501	U2F	C1-O1-PB-O3A
2	C	501	U2F	PA-O3A-PB-O2B
3	B	502	T83	CAJ-CAK-OAH-CAA
2	D	501	U2F	C5'-O5'-PA-O3A
2	A	501	U2F	PA-O3A-PB-O1B
2	D	501	U2F	PA-O3A-PB-O2B
2	C	501	U2F	C5'-O5'-PA-O2A
2	D	501	U2F	C5'-O5'-PA-O2A
2	A	501	U2F	O4'-C4'-C5'-O5'
2	B	501	U2F	O4'-C4'-C5'-O5'

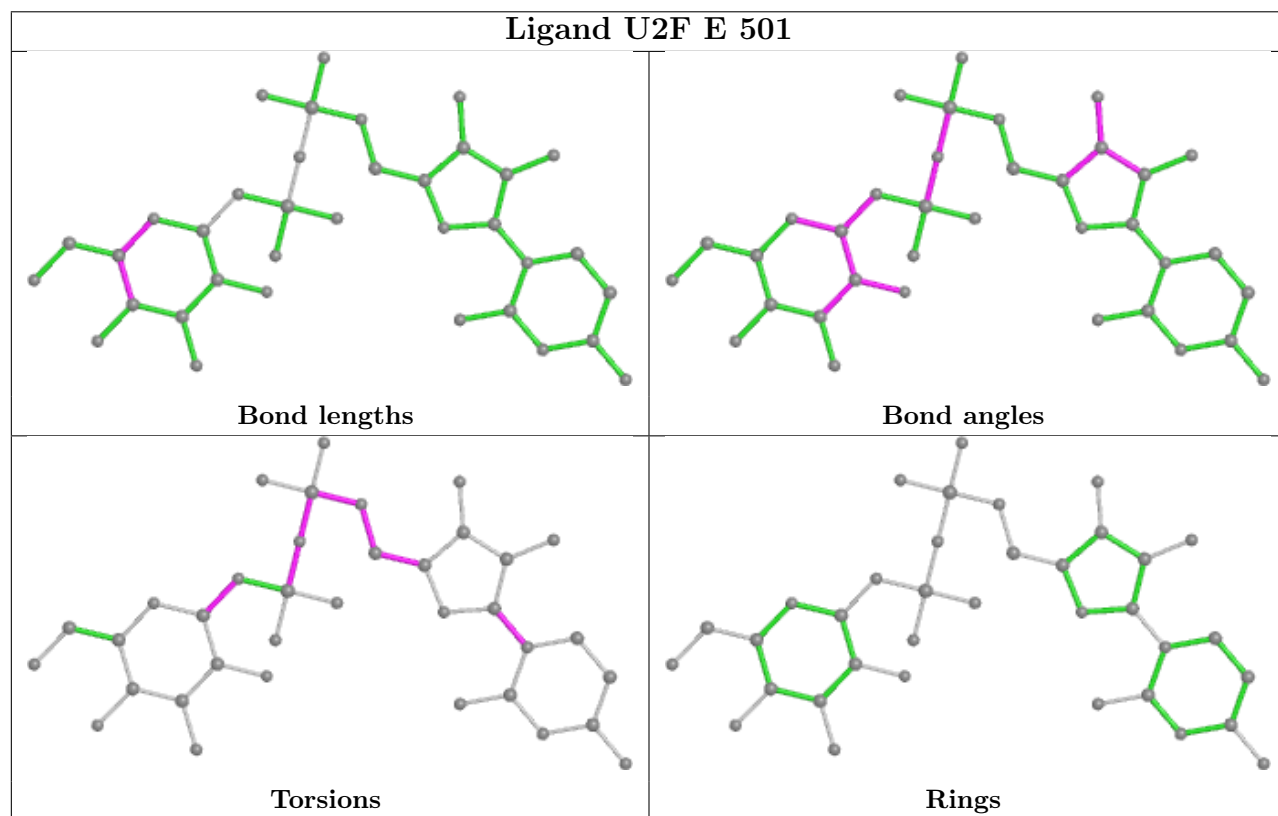
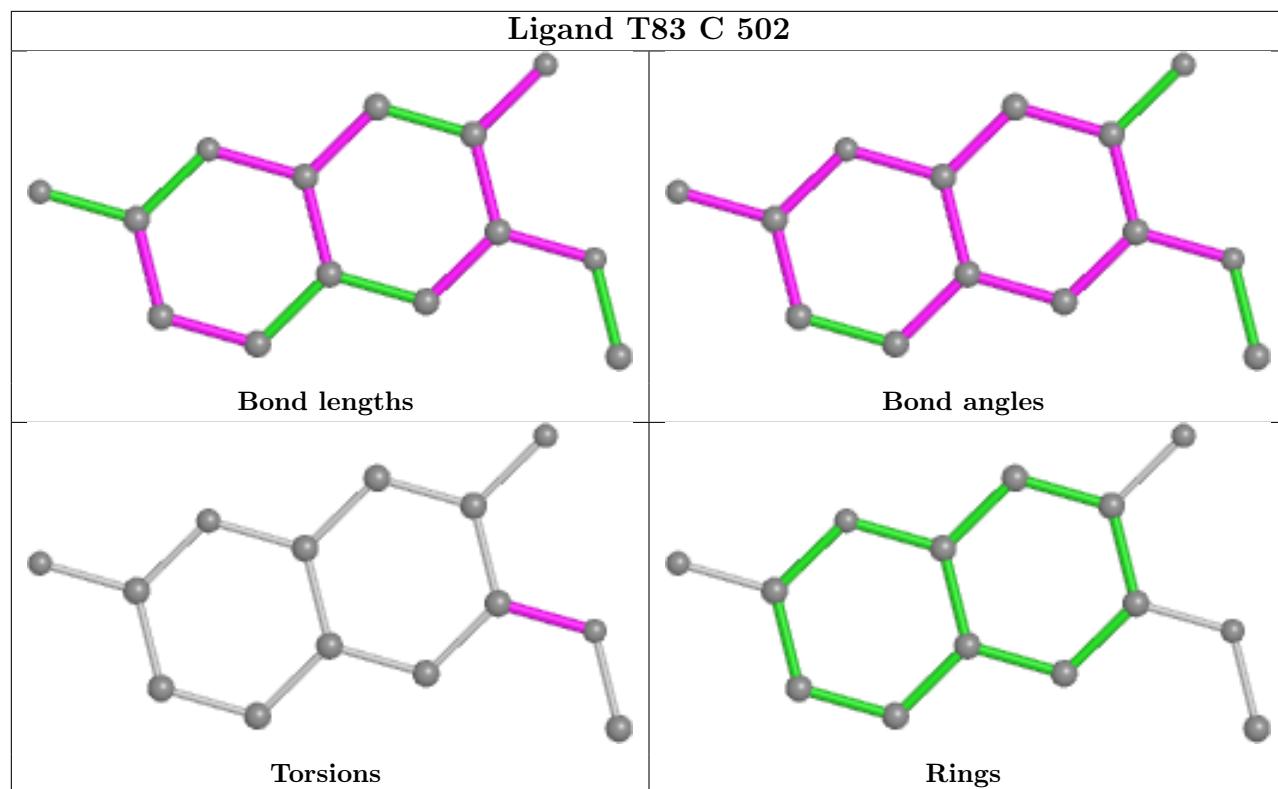
There are no ring outliers.

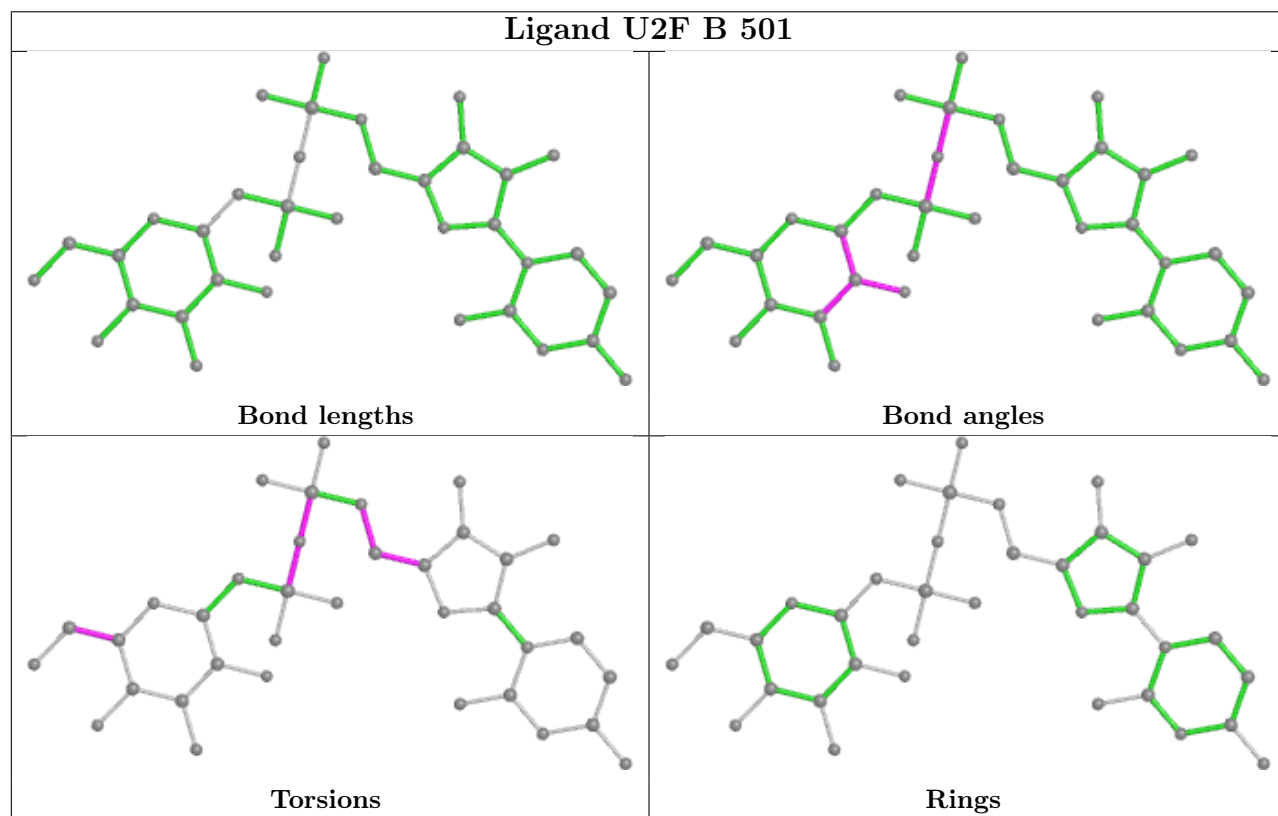
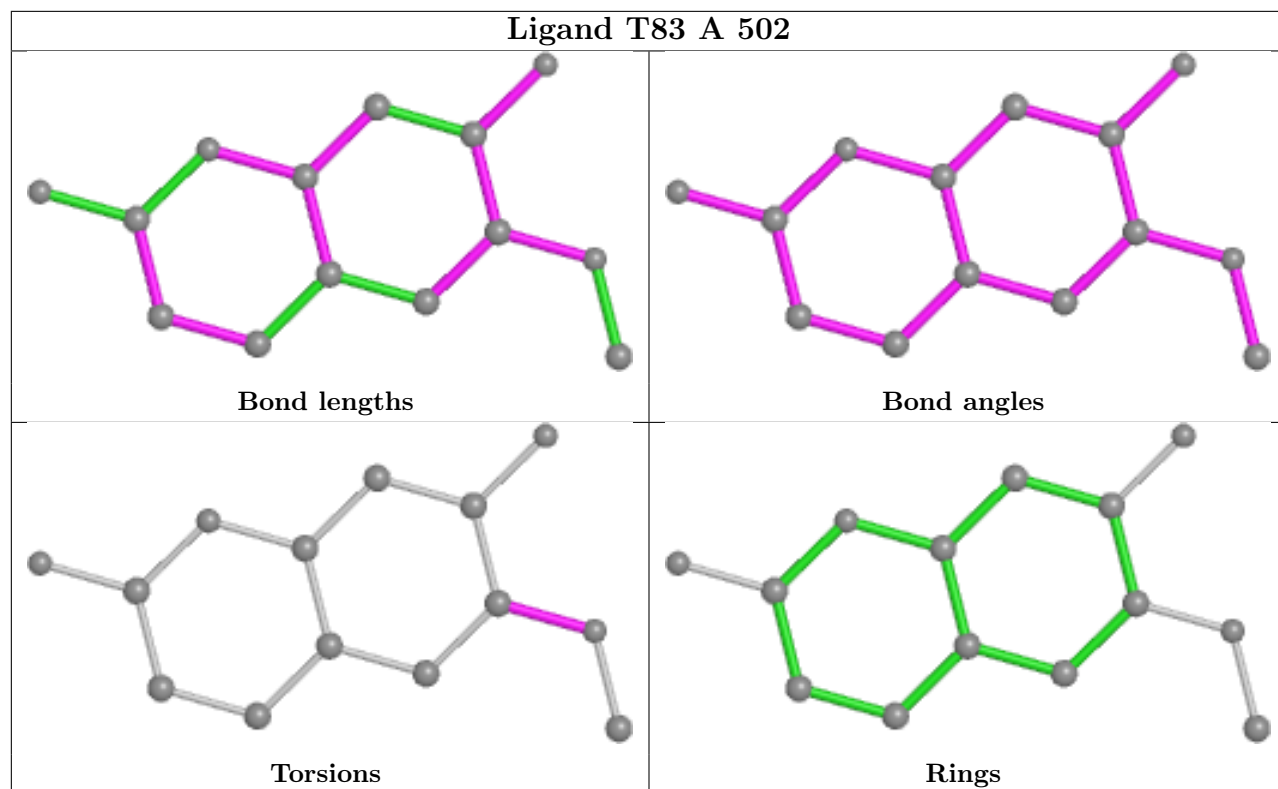
10 monomers are involved in 97 short contacts:

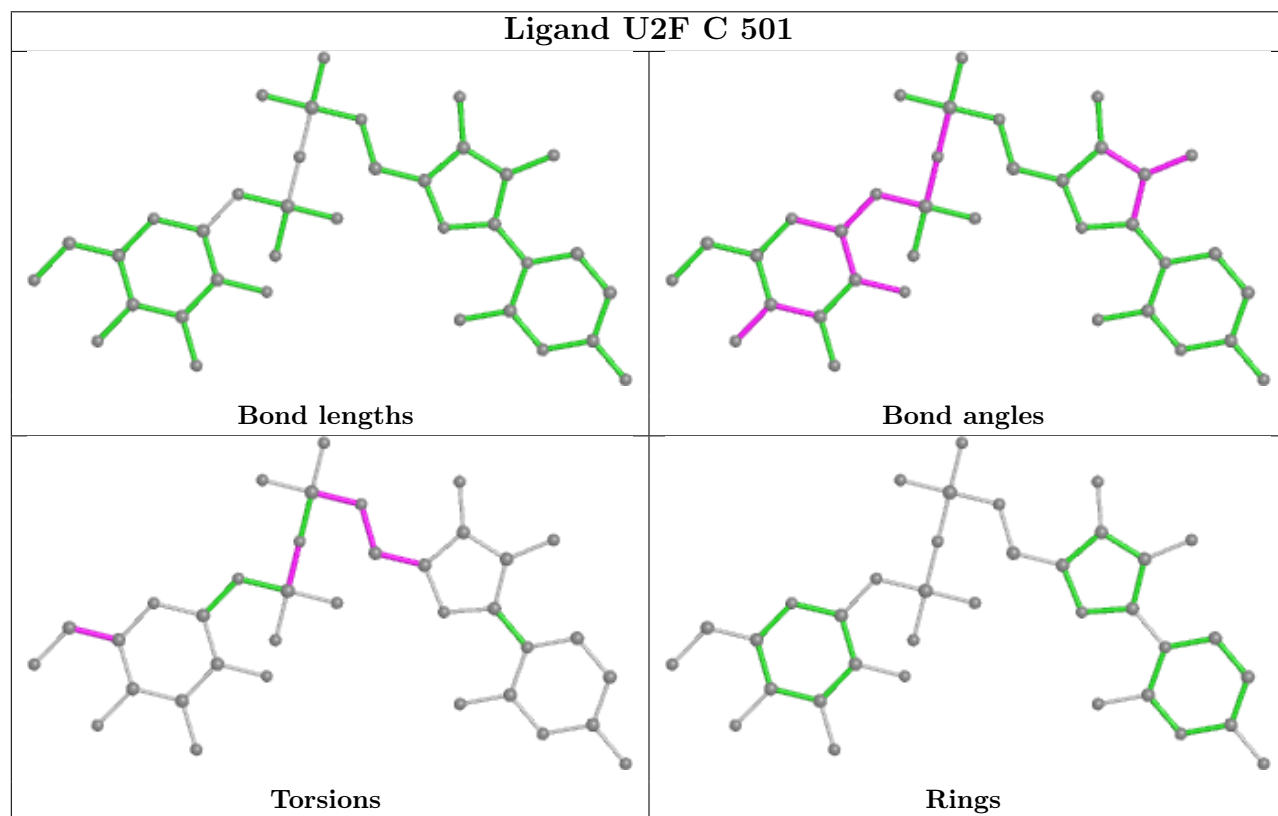
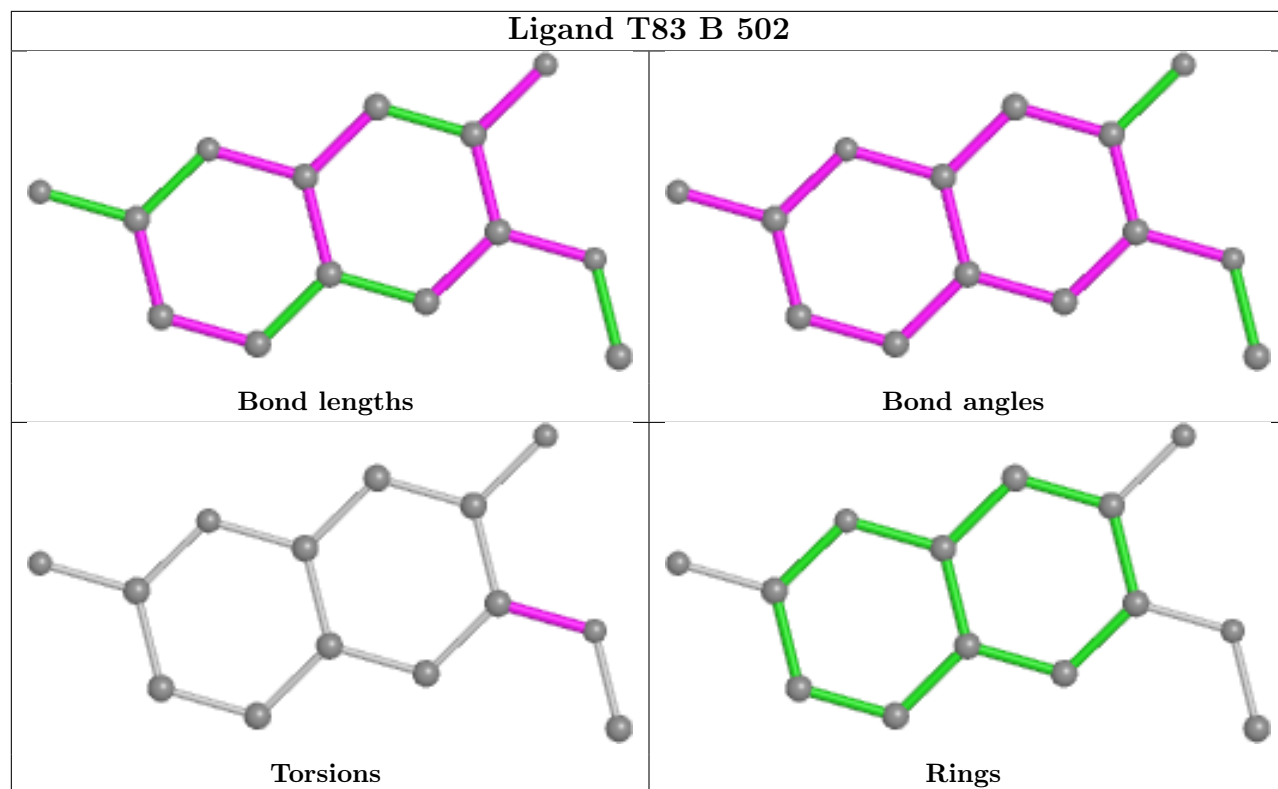
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	U2F	11	0
2	G	501	U2F	9	0
3	C	502	T83	1	0
2	E	501	U2F	15	0
3	A	502	T83	3	0
2	B	501	U2F	8	0
2	C	501	U2F	36	0
2	F	501	U2F	7	0
2	A	501	U2F	11	0
3	D	502	T83	1	0

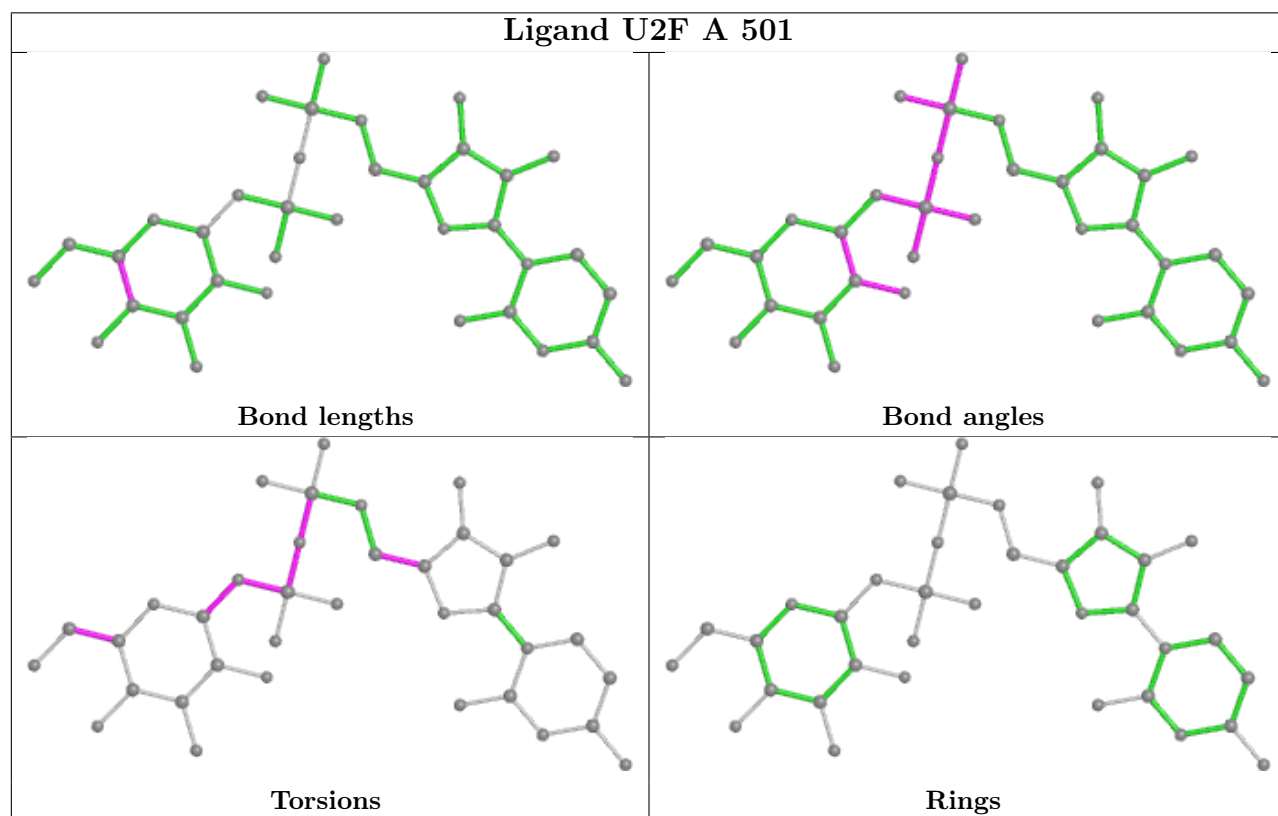
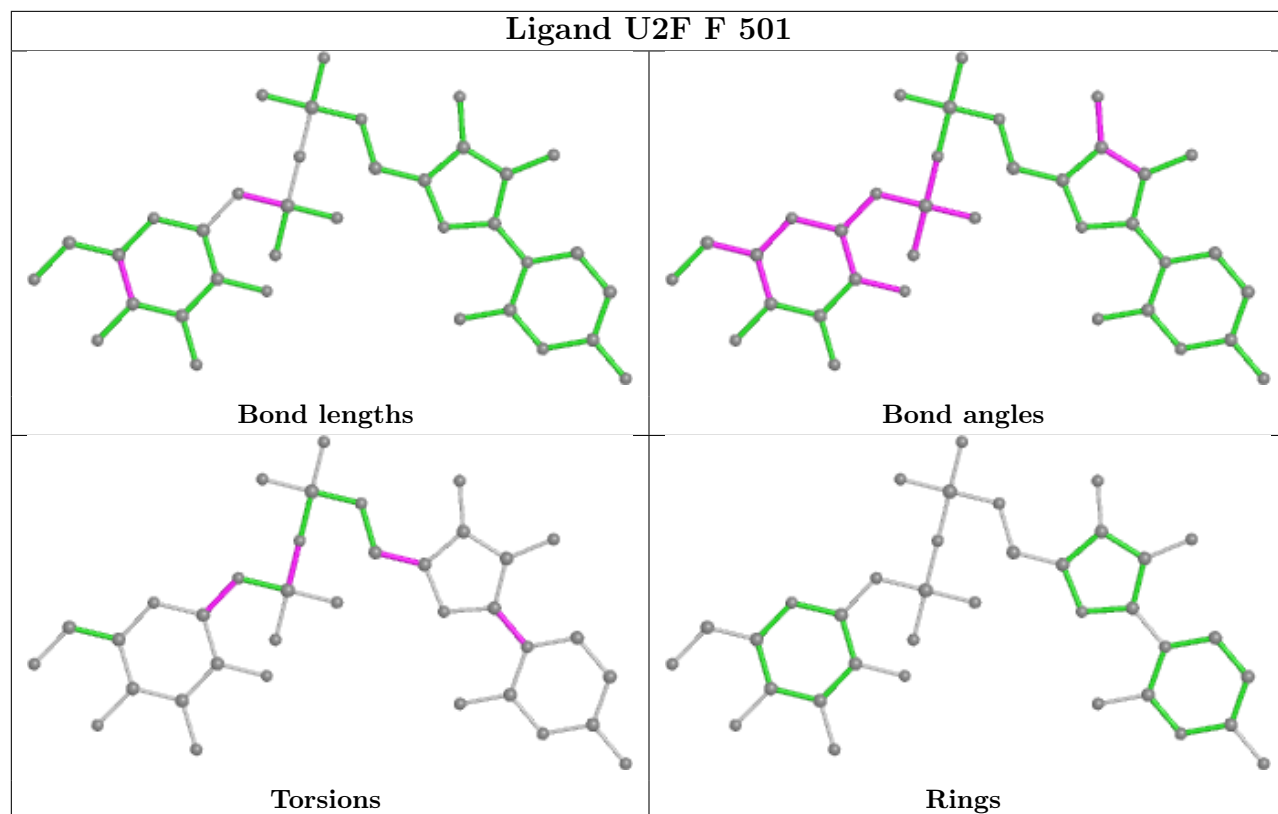
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

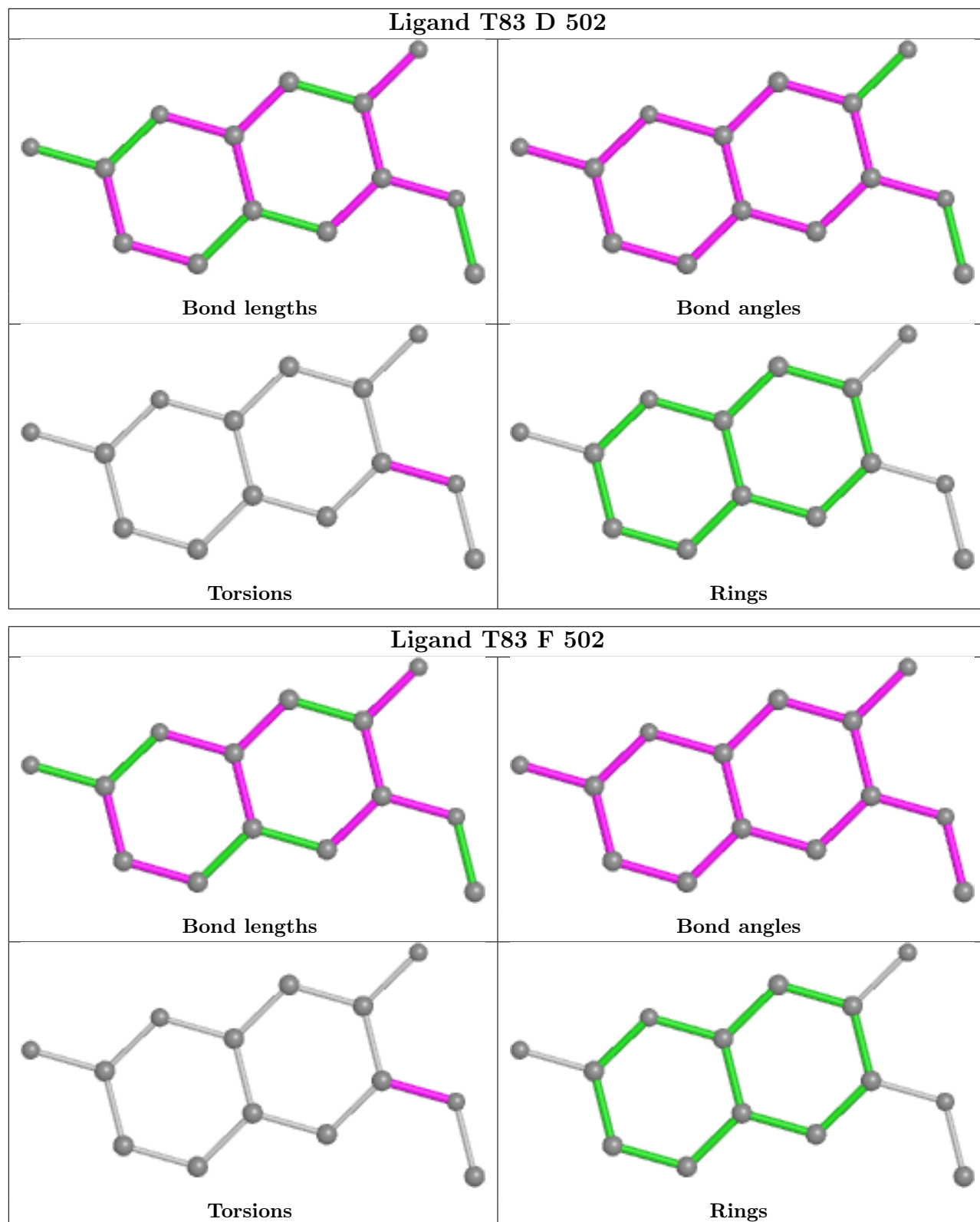












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	458/482 (95%)	0.44	22 (4%) 30 28	30, 103, 130, 147	0
1	B	460/482 (95%)	0.47	21 (4%) 32 30	30, 101, 115, 124	0
1	C	460/482 (95%)	0.56	30 (6%) 18 18	30, 105, 130, 142	0
1	D	459/482 (95%)	0.50	23 (5%) 28 26	93, 107, 122, 133	0
1	E	459/482 (95%)	0.67	39 (8%) 10 10	96, 112, 139, 160	0
1	F	460/482 (95%)	0.55	29 (6%) 20 19	92, 109, 130, 148	0
1	G	460/482 (95%)	0.72	61 (13%) 3 3	30, 129, 175, 192	0
All	All	3216/3374 (95%)	0.56	225 (6%) 16 15	30, 108, 143, 192	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	256	ASN	9.3
1	G	66	ILE	7.8
1	A	63	GLU	7.0
1	E	349	MET	5.9
1	F	227	LEU	5.8
1	G	67	GLU	5.6
1	E	325	THR	5.1
1	B	160	GLU	5.0
1	G	255	LEU	5.0
1	C	76	ILE	5.0
1	C	75	ASP	4.9
1	G	54	LEU	4.9
1	F	163	TYR	4.9
1	G	165	GLU	4.7
1	C	325	THR	4.6
1	E	477	LEU	4.6
1	G	38	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	F	205	TYR	4.5
1	D	76	ILE	4.3
1	A	273	PHE	4.3
1	F	60	THR	4.3
1	E	151	TYR	4.3
1	F	175	CYS	4.2
1	B	364	GLY	4.1
1	G	87	PHE	4.0
1	A	64	LYS	4.0
1	E	233	LEU	4.0
1	E	164	VAL	3.9
1	A	274	VAL	3.7
1	G	143	ALA	3.7
1	B	65	THR	3.7
1	G	92	LEU	3.6
1	E	6	LEU	3.6
1	E	173	PRO	3.6
1	C	280	GLY	3.6
1	G	365	PHE	3.6
1	G	80	ILE	3.6
1	G	282	LEU	3.5
1	G	65	THR	3.5
1	C	186	PRO	3.5
1	C	404	LEU	3.5
1	E	186	PRO	3.5
1	F	202	GLY	3.5
1	E	90	LEU	3.5
1	D	236	LEU	3.4
1	F	122	THR	3.4
1	E	172	ILE	3.4
1	C	328	MET	3.4
1	F	273	PHE	3.4
1	G	110	HIS	3.3
1	E	227	LEU	3.3
1	G	63	GLU	3.3
1	D	362	VAL	3.3
1	G	240	PRO	3.3
1	E	257	ASP	3.3
1	E	214	ASN	3.2
1	D	78	HIS	3.2
1	C	147	ALA	3.2
1	A	137	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	251	VAL	3.1
1	G	42	ILE	3.1
1	C	422	GLU	3.1
1	E	281	THR	3.1
1	C	241	VAL	3.1
1	G	329	SER	3.1
1	E	76	ILE	3.0
1	D	163	TYR	3.0
1	F	65	THR	3.0
1	G	113	ASP	3.0
1	F	477	LEU	3.0
1	F	303	TRP	3.0
1	B	156	ASP	3.0
1	G	133	ILE	3.0
1	G	82	SER	2.9
1	A	35	ILE	2.9
1	B	227	LEU	2.9
1	E	201	LEU	2.9
1	E	387	TRP	2.9
1	G	77	SER	2.9
1	E	262	TRP	2.9
1	G	95	ARG	2.9
1	A	334	GLU	2.9
1	G	11	VAL	2.9
1	F	387	TRP	2.9
1	G	40	LEU	2.9
1	F	139	HIS	2.9
1	F	166	LEU	2.9
1	E	116	ILE	2.8
1	C	242	PHE	2.8
1	G	61	ASN	2.8
1	G	43	THR	2.8
1	G	125	LEU	2.8
1	A	159	ILE	2.8
1	B	387	TRP	2.8
1	G	62	GLU	2.8
1	E	163	TYR	2.7
1	E	343	MET	2.7
1	F	136	TYR	2.7
1	D	431	LEU	2.7
1	D	80	ILE	2.7
1	B	334	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	28	ARG	2.7
1	G	68	ILE	2.7
1	G	23	LEU	2.7
1	G	233	LEU	2.7
1	B	244	ILE	2.6
1	C	472	ILE	2.6
1	G	119	ILE	2.6
1	A	112	PRO	2.6
1	G	187	LEU	2.6
1	D	242	PHE	2.6
1	G	254	THR	2.6
1	D	233	LEU	2.6
1	G	333	PRO	2.6
1	F	408	ILE	2.6
1	G	96	GLU	2.6
1	E	336	PHE	2.5
1	E	294	LEU	2.5
1	A	336	PHE	2.5
1	D	53	PHE	2.5
1	G	207	ASP	2.5
1	F	86	ILE	2.5
1	A	134	SER	2.5
1	G	32	HIS	2.5
1	E	83	SER	2.5
1	D	237	LEU	2.5
1	C	352	ASN	2.5
1	G	428	VAL	2.5
1	B	299	GLN	2.5
1	E	205	TYR	2.4
1	C	199	VAL	2.4
1	D	150	ILE	2.4
1	E	101	ILE	2.4
1	G	302	VAL	2.4
1	F	151	TYR	2.4
1	F	39	ILE	2.4
1	C	14	PRO	2.4
1	E	388	PRO	2.4
1	D	301	PHE	2.4
1	G	117	VAL	2.4
1	A	65	THR	2.4
1	F	87	PHE	2.4
1	G	476	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	124	ILE	2.4
1	C	227	LEU	2.4
1	E	40	LEU	2.4
1	G	424	ILE	2.4
1	B	79	LEU	2.4
1	A	381	GLY	2.3
1	A	352	ASN	2.3
1	B	404	LEU	2.3
1	F	79	LEU	2.3
1	B	363	GLY	2.3
1	F	33	HIS	2.3
1	C	228	ARG	2.3
1	A	477	LEU	2.3
1	C	224	ILE	2.3
1	E	471	ASP	2.3
1	F	170	LEU	2.3
1	B	113	ASP	2.3
1	G	406	VAL	2.3
1	F	307	PRO	2.3
1	C	110	HIS	2.3
1	A	205	TYR	2.3
1	D	387	TRP	2.3
1	A	27	ASN	2.3
1	G	191	SER	2.3
1	C	168	GLU	2.2
1	G	345	LEU	2.2
1	G	112	PRO	2.2
1	E	340	THR	2.2
1	G	205	TYR	2.2
1	D	116	ILE	2.2
1	B	253	THR	2.2
1	C	40	LEU	2.2
1	D	6	LEU	2.2
1	A	87	PHE	2.2
1	D	276	PHE	2.2
1	D	205	TYR	2.2
1	E	344	GLY	2.2
1	A	227	LEU	2.2
1	D	87	PHE	2.2
1	A	11	VAL	2.2
1	C	184	VAL	2.2
1	E	150	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	308	PRO	2.2
1	C	214	ASN	2.2
1	C	362	VAL	2.2
1	C	146	LEU	2.1
1	F	219	LEU	2.1
1	B	388	PRO	2.1
1	G	115	LEU	2.1
1	E	177	ALA	2.1
1	G	175	CYS	2.1
1	G	273	PHE	2.1
1	C	119	ILE	2.1
1	G	105	ILE	2.1
1	D	187	LEU	2.1
1	A	93	LEU	2.1
1	A	384	MET	2.1
1	G	307	PRO	2.1
1	B	362	VAL	2.1
1	C	89	GLN	2.1
1	B	185	ASP	2.1
1	C	172	ILE	2.1
1	B	233	LEU	2.1
1	G	116	ILE	2.1
1	C	115	LEU	2.1
1	G	46	SER	2.1
1	C	62	GLU	2.0
1	E	175	CYS	2.0
1	D	398	ALA	2.0
1	F	274	VAL	2.0
1	E	378	LEU	2.0
1	F	96	GLU	2.0
1	D	177	ALA	2.0
1	E	26	GLY	2.0
1	G	131	PHE	2.0
1	G	33	HIS	2.0
1	F	190	ARG	2.0
1	G	127	ILE	2.0
1	B	353	GLN	2.0
1	B	39	ILE	2.0
1	B	159	ILE	2.0
1	G	178	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](#)

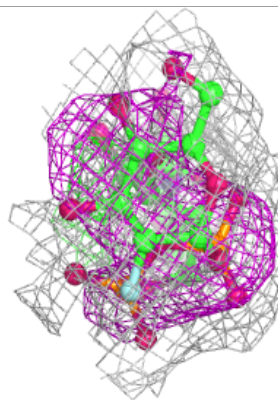
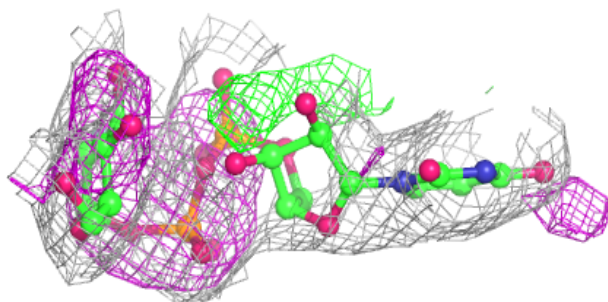
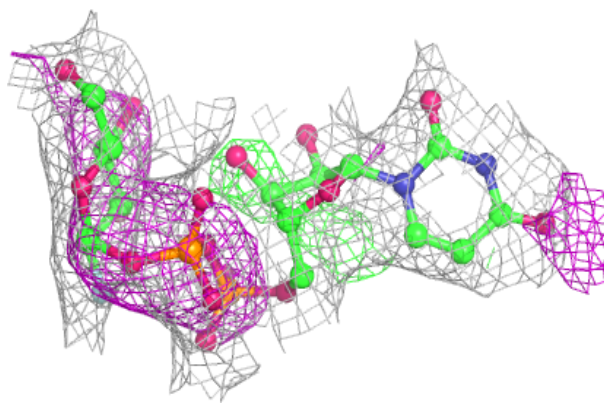
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	U2F	C	501	36/36	0.83	0.23	46,46,46,46	0
3	T83	A	502	14/14	0.86	0.75	46,46,46,46	0
2	U2F	E	501	36/36	0.87	0.25	46,46,46,46	0
3	T83	B	502	14/14	0.89	0.56	46,46,46,46	0
3	T83	F	502	14/14	0.90	0.34	46,46,46,46	0
3	T83	C	502	14/14	0.91	0.58	46,46,46,46	0
3	T83	D	502	14/14	0.91	0.65	46,46,46,46	0
2	U2F	F	501	36/36	0.91	0.21	46,46,46,46	0
2	U2F	G	501	36/36	0.92	0.17	46,46,46,46	0
2	U2F	A	501	36/36	0.92	0.20	46,46,46,46	0
2	U2F	B	501	36/36	0.93	0.21	46,46,46,46	0
2	U2F	D	501	36/36	0.94	0.20	46,46,46,46	0

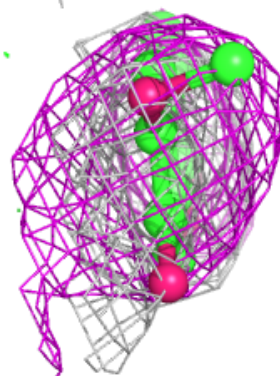
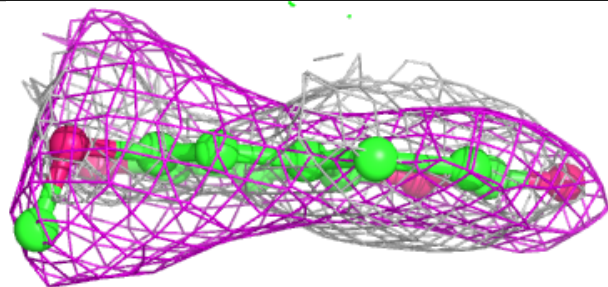
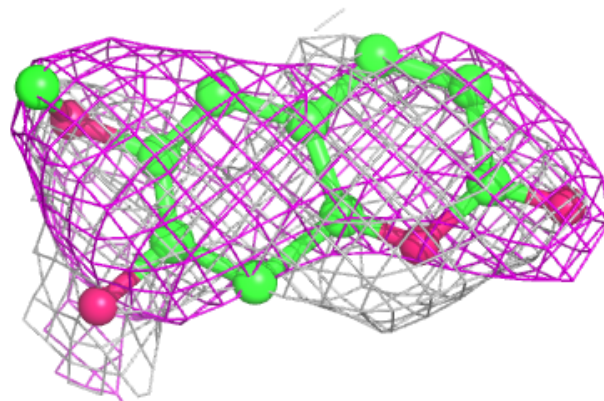
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around U2F C 501:

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

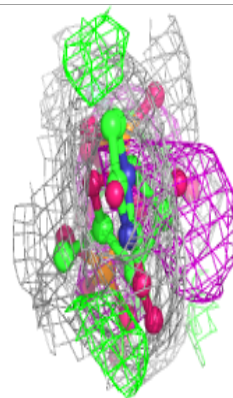
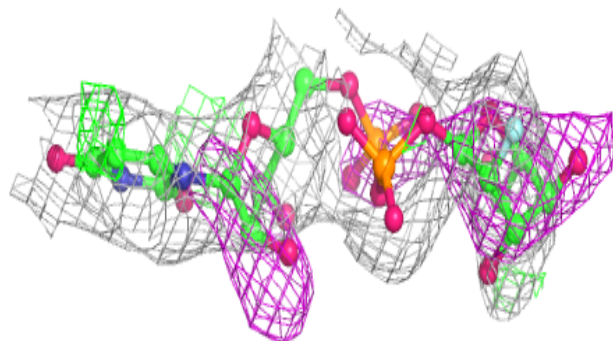
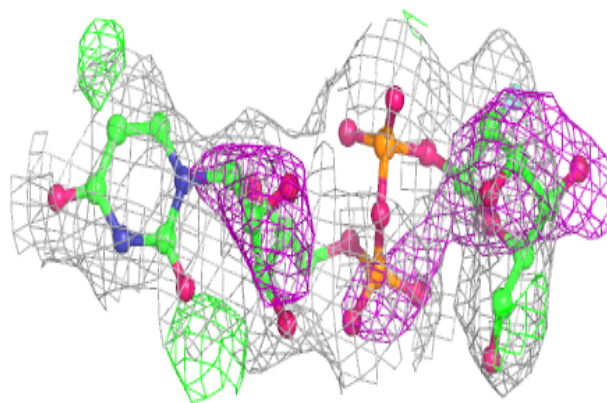
**Electron density around T83 A 502:**

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



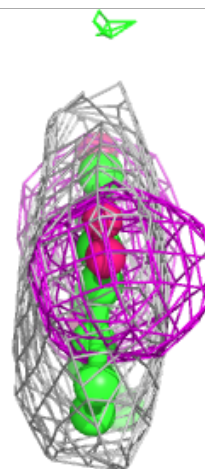
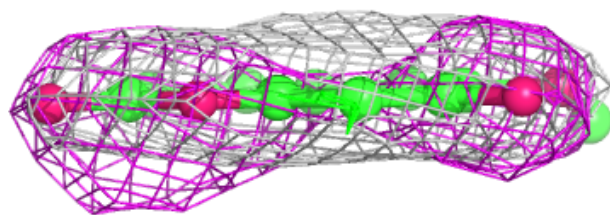
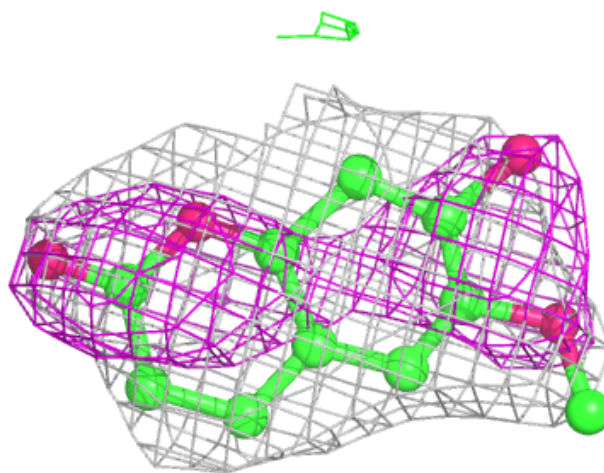
Electron density around U2F E 501:

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



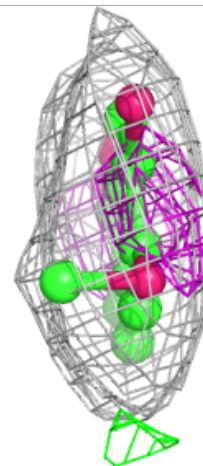
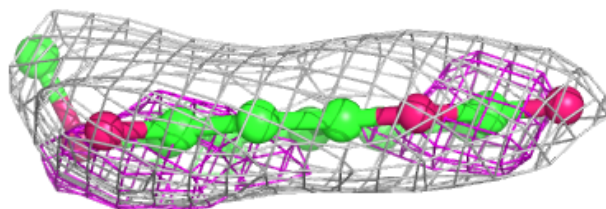
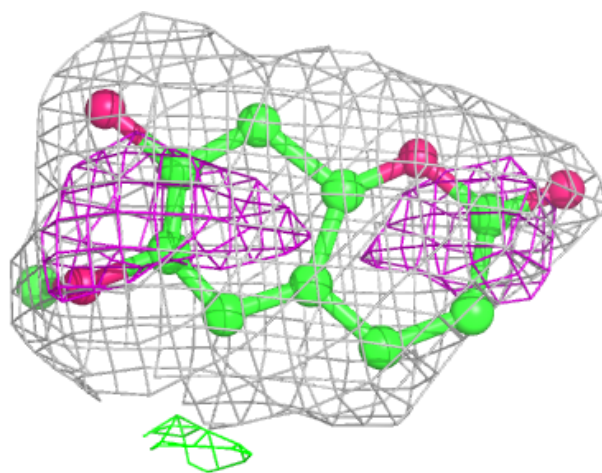
Electron density around T83 B 502:

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



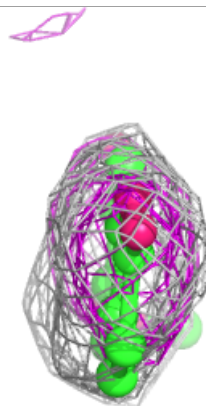
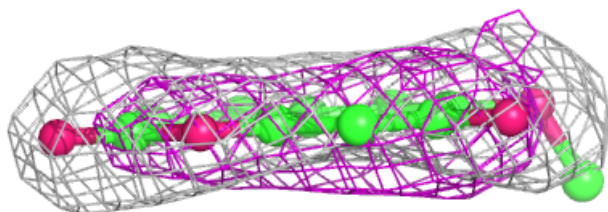
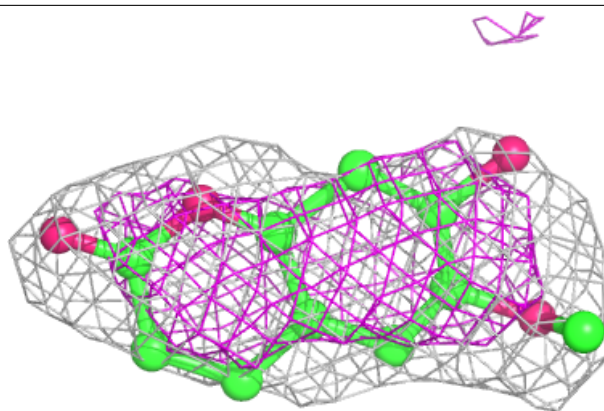
Electron density around T83 F 502:

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

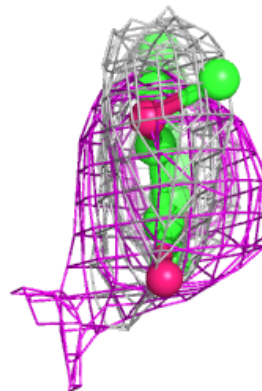
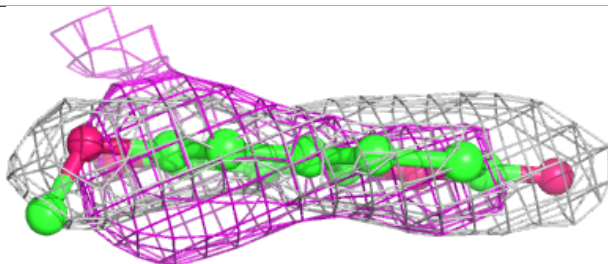
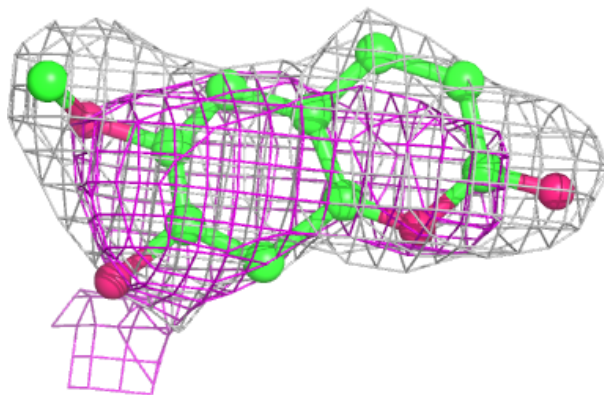


Electron density around T83 C 502:

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

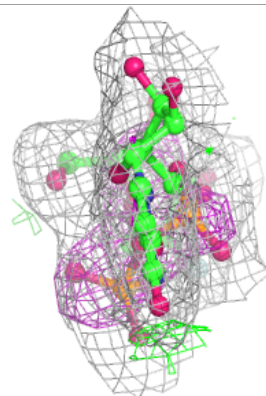
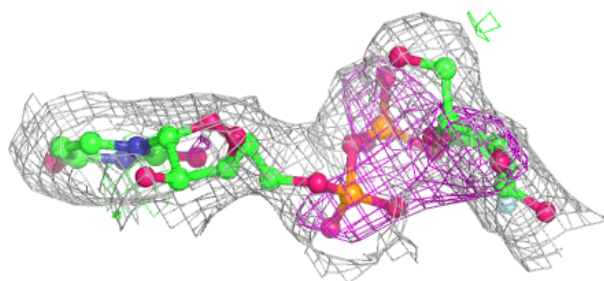
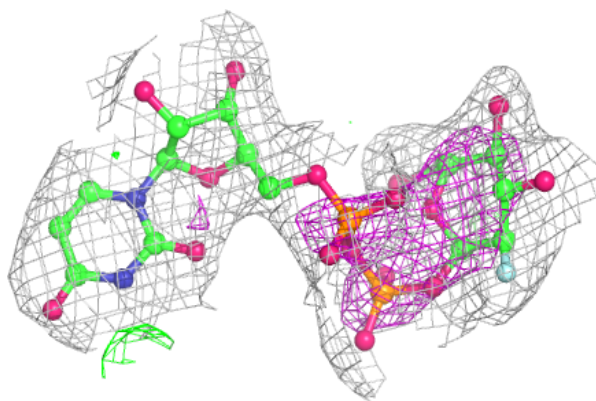
**Electron density around T83 D 502:**

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

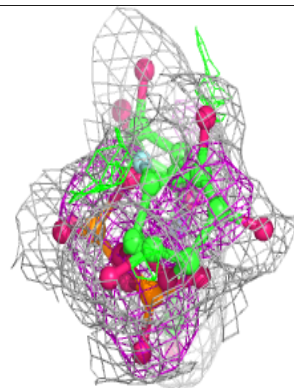
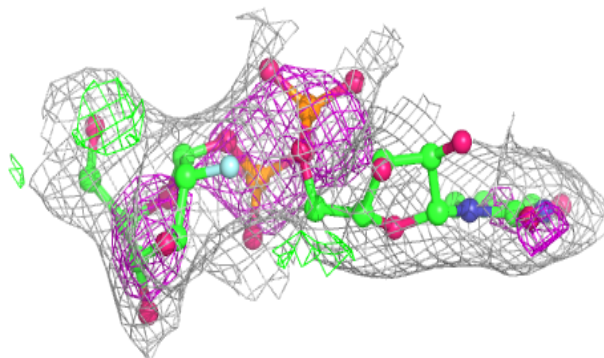
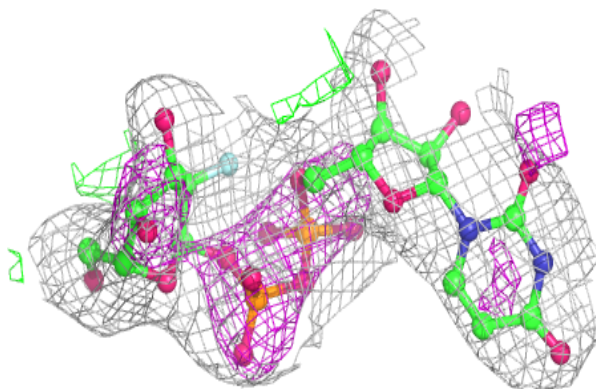


Electron density around U2F F 501:

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

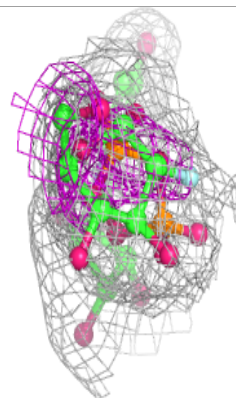
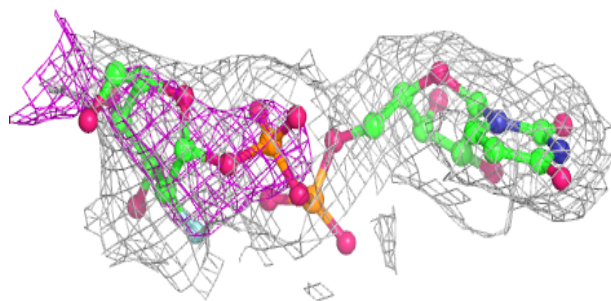
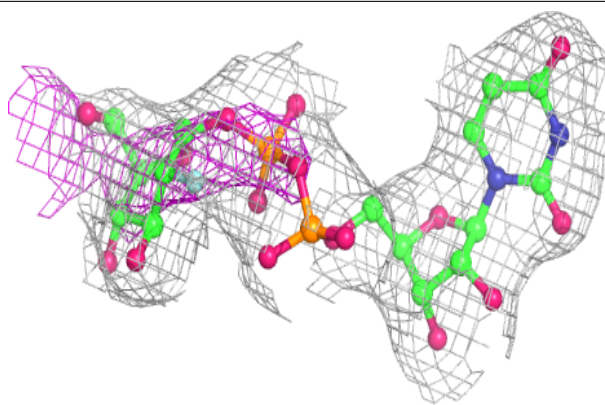
**Electron density around U2F G 501:**

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

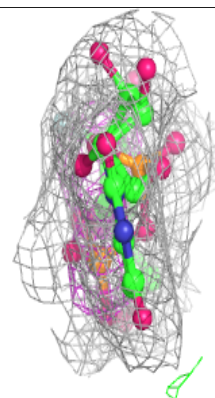
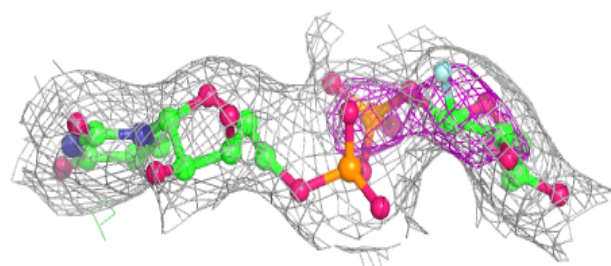
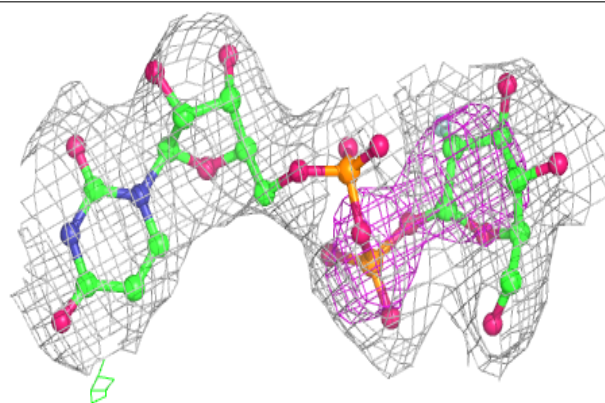


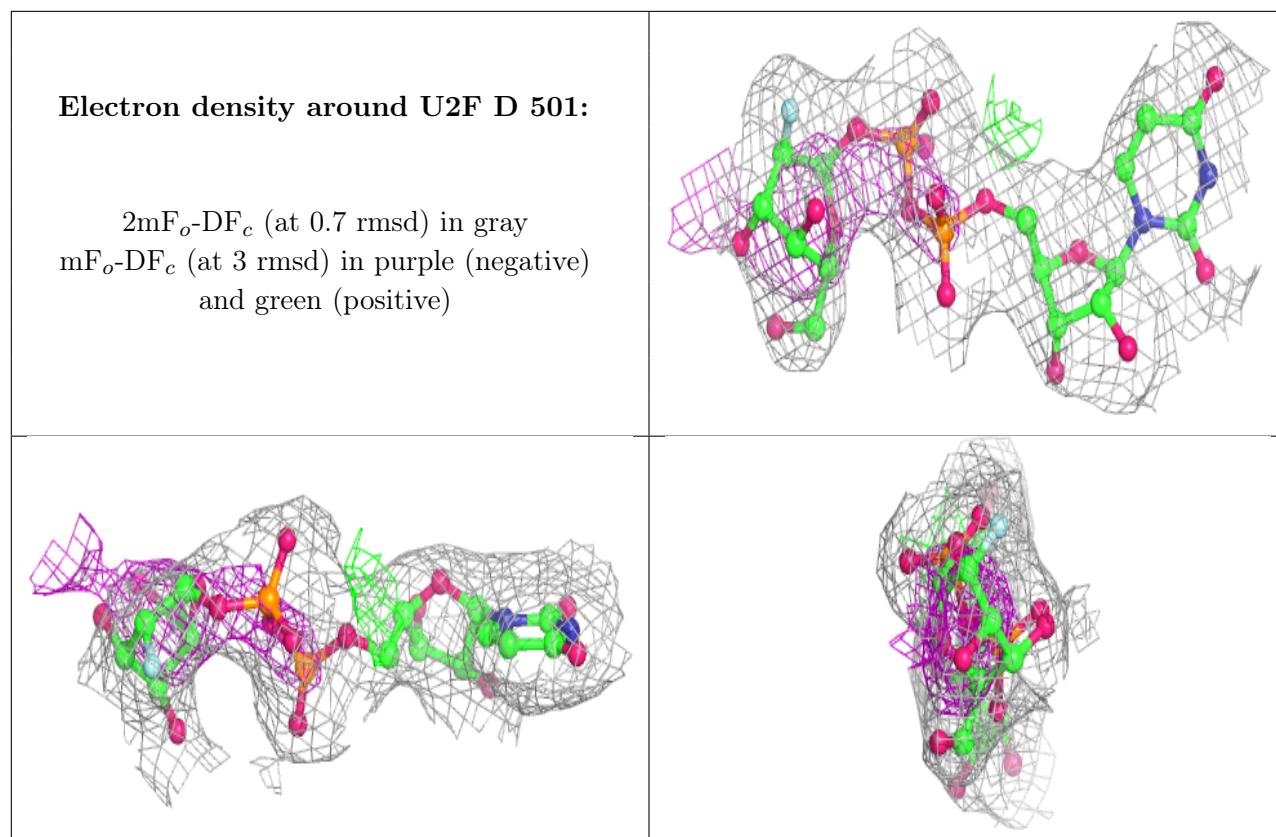
Electron density around U2F A 501:

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

**Electron density around U2F B 501:**

$2mF_o-DF_c$ (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.