



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:50 PM UTC

PDB ID : 9LRJ / pdb_00009lrj
Title : Glucosyl transferase NbUGT72AY1 co-crystallized with Scopoletin and UDP2Fglucose in the presence of retinol
Authors : Arold, S.T.; Hameed, U.F.S.
Deposited on : 2025-01-31
Resolution : 3.11 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

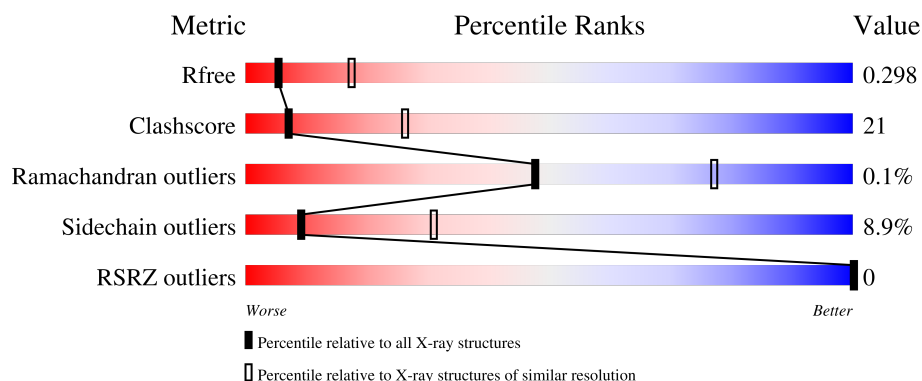
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.11 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}	180053	1816 (3.14-3.10)
Clashscore	190562	1906 (3.14-3.10)
Ramachandran outliers	187476	1802 (3.14-3.10)
Sidechain outliers	187428	1802 (3.14-3.10)
RSRZ outliers	180081	1816 (3.14-3.10)

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	479	
1	B	479	
1	C	479	
1	D	479	
1	E	479	

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Mol	Chain	Length	Quality of chain
1	F	479	
1	G	479	

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	C	501	-	-	X	-
2	U2F	E	501	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25741 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
1	A	455	Total	C	N	O	S	0	0	0
			3600	2302	605	677	16			
1	B	459	Total	C	N	O	S	0	0	0
			3633	2321	611	685	16			
1	C	460	Total	C	N	O	S	0	0	0
			3640	2325	612	687	16			
1	D	460	Total	C	N	O	S	0	0	0
			3640	2325	612	687	16			
1	E	459	Total	C	N	O	S	0	0	0
			3633	2321	611	685	16			
1	F	459	Total	C	N	O	S	0	0	0
			3633	2321	611	685	16			
1	G	460	Total	C	N	O	S	0	0	0
			3640	2325	612	687	16			

There are 28 discrepancies between the modelled and reference sequences:

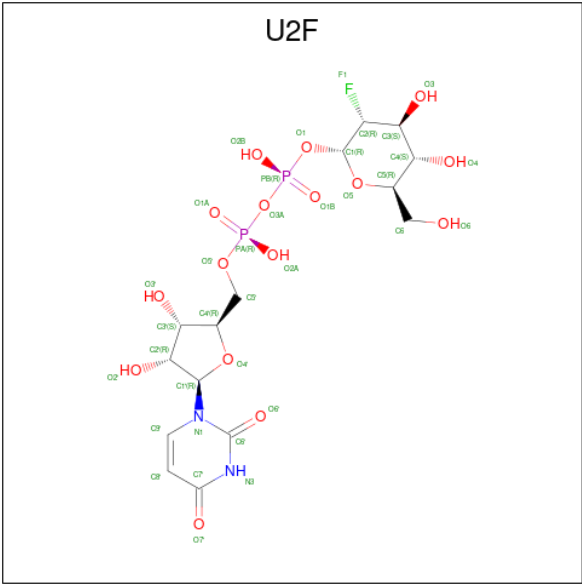
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
A	0	PRO	-	expression tag	UNP A0A8K1ZRH3
A	1	LEU	-	expression tag	UNP A0A8K1ZRH3
A	2	GLY	-	expression tag	UNP A0A8K1ZRH3
B	-1	GLY	-	expression tag	UNP A0A8K1ZRH3
B	0	PRO	-	expression tag	UNP A0A8K1ZRH3
B	1	LEU	-	expression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

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

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



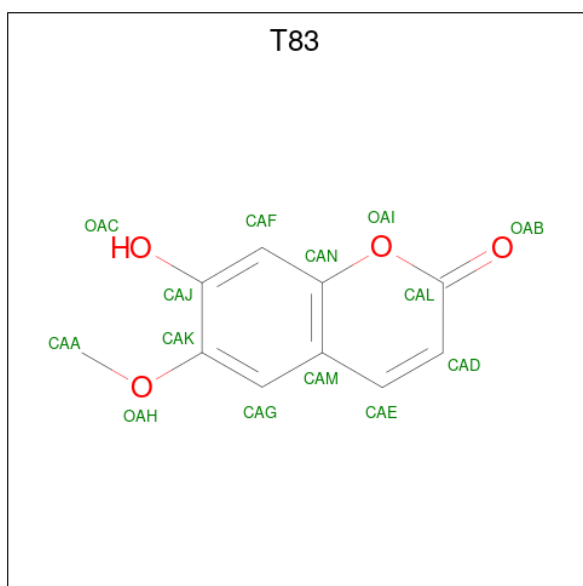
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	B	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	C	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		
2	D	1	Total	C	F	N	O	P	0	0
			36	15	1	2	16	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
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 (CCD ID: T83) (formula: $C_{10}H_8O_4$) (labeled as "Ligand of Interest" by depositor).

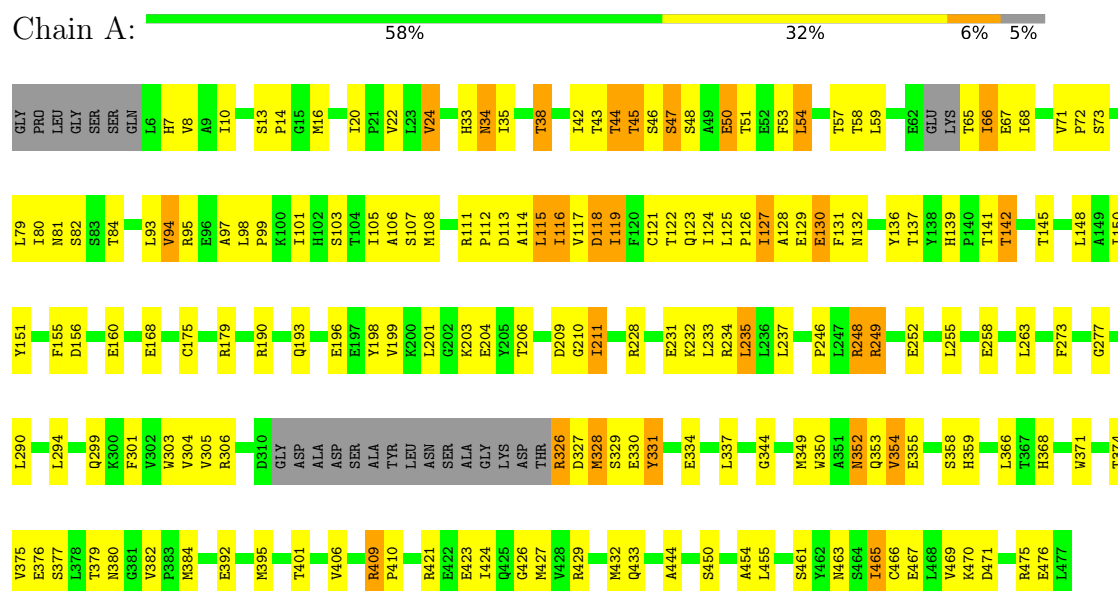


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			14	10	4		
3	B	1	Total	C	O	0	0
			14	10	4		
3	C	1	Total	C	O	0	0
			14	10	4		
3	D	1	Total	C	O	0	0
			14	10	4		
3	F	1	Total	C	O	0	0
			14	10	4		

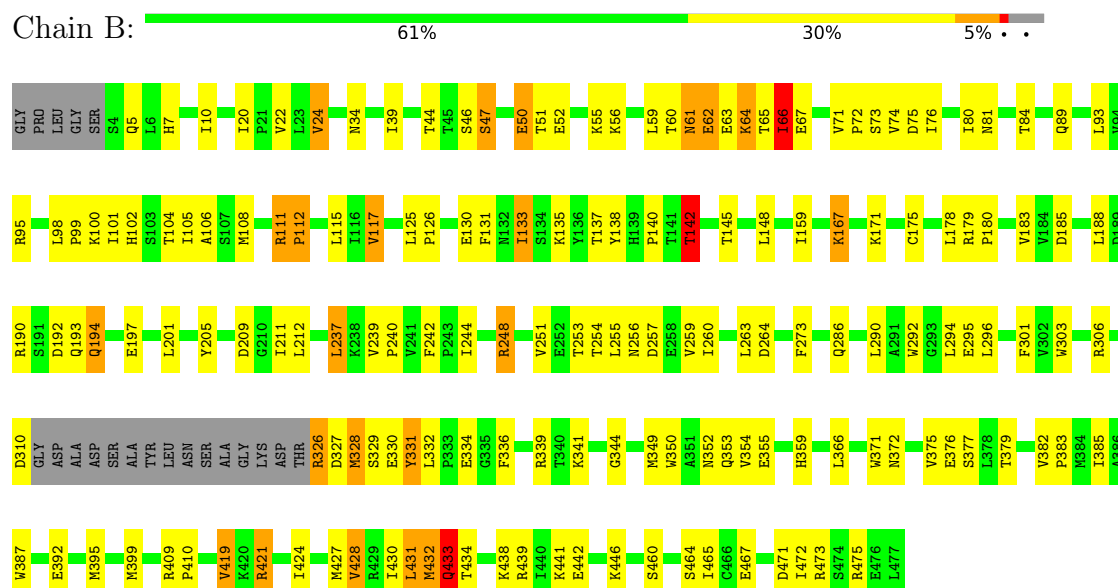
3 Residue-property plots

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

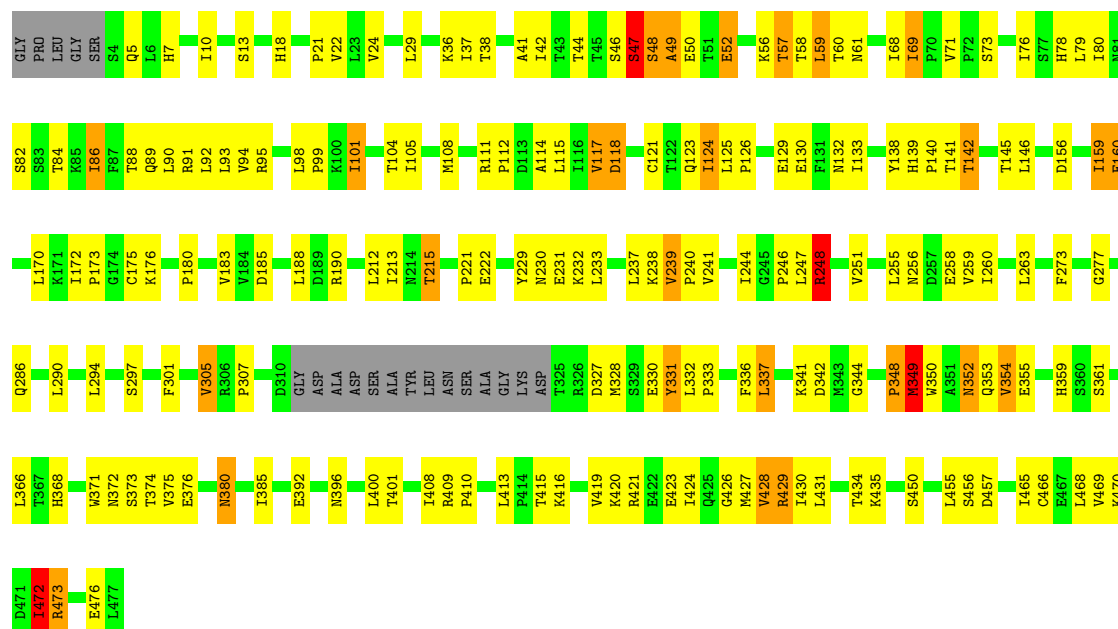


• Molecule 1: Glycosyltransferase



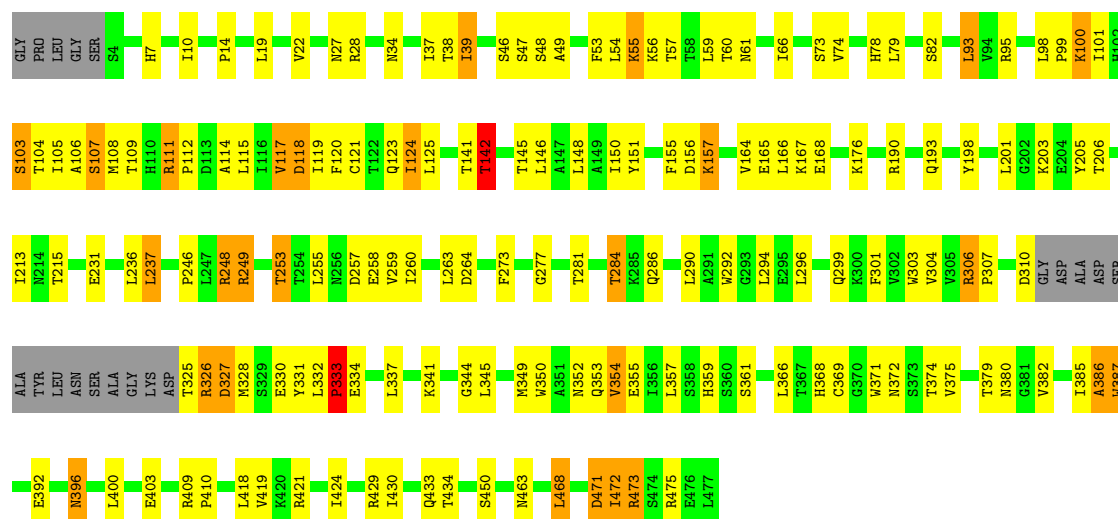
- Molecule 1: Glycosyltransferase

Chain C:  57% 33% 5% . .



- Molecule 1: Glycosyltransferase

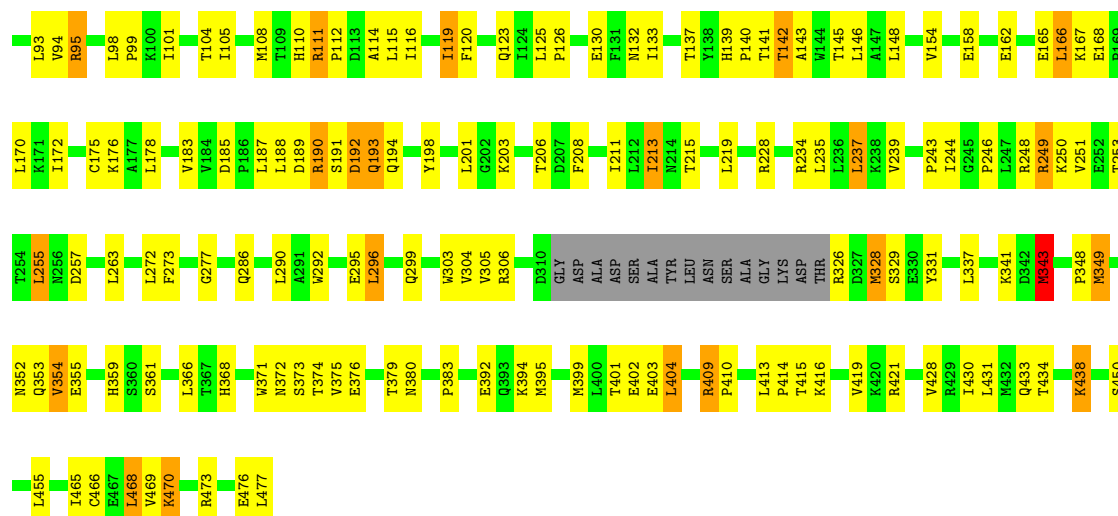
Chain D:  62% 28% 6% .



- Molecule 1: Glycosyltransferase

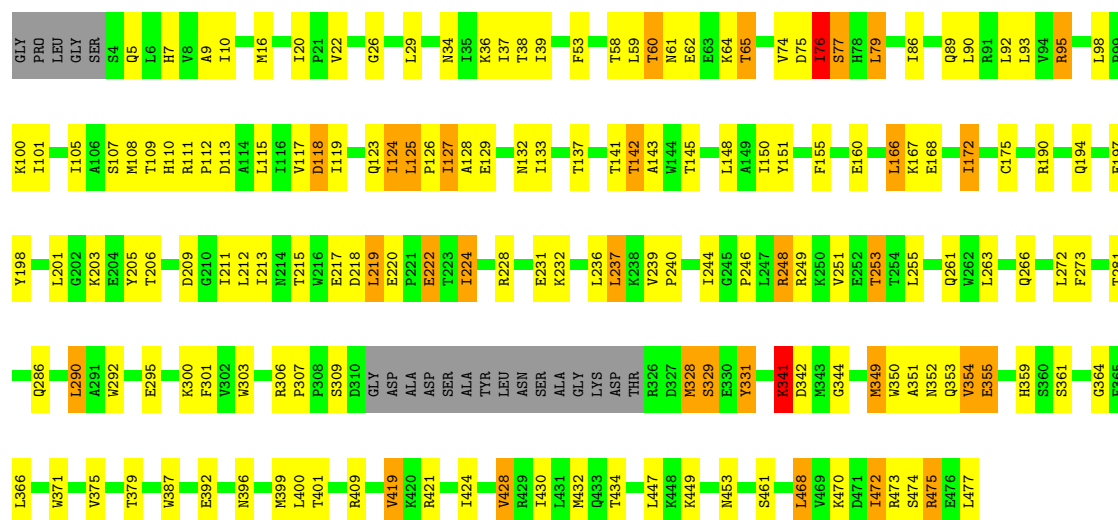
Chain E:  57% 33% 5% .





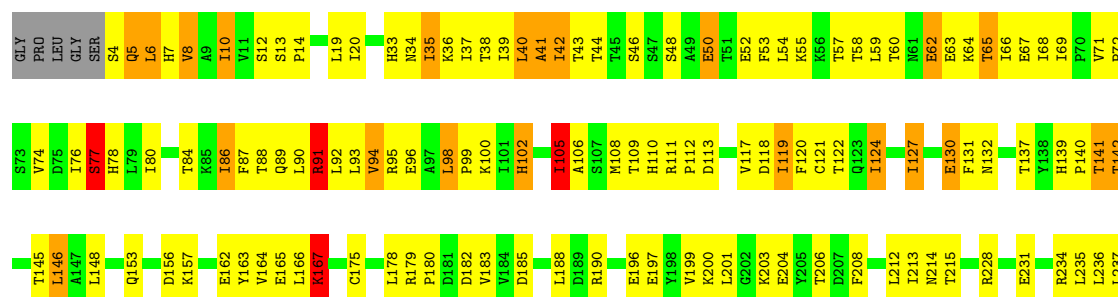
• Molecule 1: Glycosyltransferase

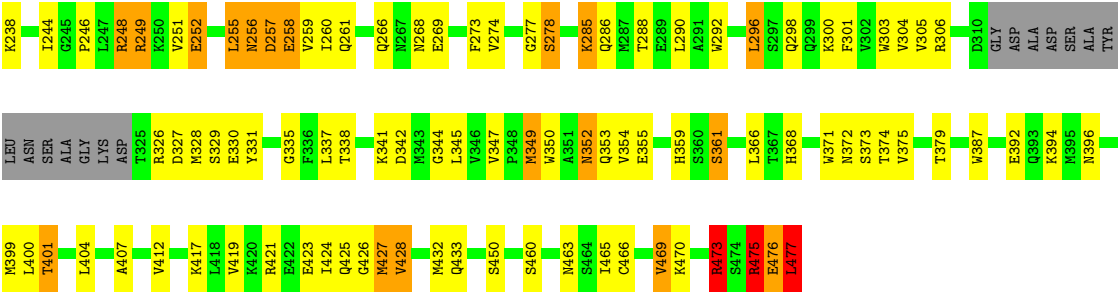
Chain F: 61% 28% 6%



• Molecule 1: Glycosyltransferase

Chain G: 49% 37% 8%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.72Å 171.78Å 153.38Å 90.00° 93.35° 90.00°	Depositor
Resolution (Å)	48.89 – 3.11 48.89 – 3.11	Depositor EDS
% Data completeness (in resolution range)	68.8 (48.89-3.11) 58.2 (48.89-3.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.12Å)	Xtriage
Refinement program	REFMAC Refmac5	Depositor
R, R_{free}	0.268 , 0.312 0.264 , 0.298	Depositor DCC
R_{free} test set	2878 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtriage
Anisotropy	0.308	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 76.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25741	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.68	0/3670	1.15	19/4978 (0.4%)
1	B	0.67	0/3704	1.31	36/5024 (0.7%)
1	C	0.69	1/3711 (0.0%)	1.23	25/5034 (0.5%)
1	D	0.66	1/3711 (0.0%)	1.18	27/5034 (0.5%)
1	E	0.68	0/3704	1.18	19/5024 (0.4%)
1	F	0.66	0/3704	1.21	20/5024 (0.4%)
1	G	0.73	0/3711	1.38	42/5034 (0.8%)
All	All	0.68	2/25915 (0.0%)	1.24	188/35152 (0.5%)

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	8
1	C	0	6
1	D	0	8
1	E	0	10
1	F	0	7
1	G	0	9
All	All	0	57

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	231	GLU	C-O	-11.06	1.09	1.24
1	D	387	TRP	N-CA	5.51	1.50	1.46

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	59	LEU	CB-CA-C	-25.61	72.85	111.77
1	E	192	ASP	N-CA-C	21.95	141.39	111.54
1	C	57	THR	CB-CA-C	20.93	152.07	110.42
1	B	328	MET	N-CA-C	20.19	144.98	113.28
1	D	334	GLU	N-CA-C	19.95	144.08	111.37
1	B	328	MET	CB-CA-C	-18.50	83.43	110.06
1	E	192	ASP	CB-CA-C	-18.23	85.19	111.80
1	C	348	PRO	N-CA-C	18.10	149.75	112.47
1	F	77	SER	N-CA-C	-16.57	89.91	112.12
1	B	51	THR	N-CA-C	-16.20	91.98	112.72
1	F	61	ASN	N-CA-C	15.80	129.88	111.71
1	F	128	ALA	N-CA-C	15.30	128.01	111.03
1	B	434	THR	N-CA-C	15.13	130.92	110.35
1	C	57	THR	N-CA-C	-14.20	80.56	110.80
1	G	278	SER	CB-CA-C	13.73	137.74	110.42
1	B	66	ILE	N-CA-C	-13.09	91.70	109.37
1	F	76	ILE	CB-CA-C	-12.45	90.87	111.29
1	F	60	THR	CB-CA-C	12.02	124.67	109.16
1	G	60	THR	N-CA-C	-11.86	86.83	109.24
1	B	67	GLU	N-CA-C	-11.57	89.37	108.34
1	D	333	PRO	N-CA-C	-11.36	89.07	112.47
1	B	434	THR	N-CA-CB	-11.25	93.50	110.04
1	C	58	THR	N-CA-C	-11.18	86.98	110.80
1	A	47	SER	N-CA-CB	-11.04	93.84	110.07
1	G	41	ALA	N-CA-CB	-11.02	91.13	110.86
1	B	433	GLN	CB-CA-C	10.86	132.02	110.42
1	D	255	LEU	N-CA-C	10.85	127.67	112.04
1	D	334	GLU	N-CA-CB	-10.75	91.45	109.72
1	B	47	SER	N-CA-C	10.56	133.29	110.80
1	G	66	ILE	N-CA-CB	-10.45	91.97	112.24
1	C	118	ASP	CA-CB-CG	10.44	123.04	112.60
1	G	66	ILE	N-CA-C	10.41	125.20	109.17
1	G	163	TYR	CB-CA-C	-10.39	95.09	110.06
1	B	46	SER	CB-CA-C	10.24	130.81	110.42
1	B	67	GLU	N-CA-CB	10.00	126.47	110.77
1	B	50	GLU	CB-CA-C	-9.90	91.44	110.35
1	G	476	GLU	CB-CA-C	9.90	128.28	110.16
1	A	252	GLU	N-CA-C	-9.86	90.46	108.02
1	E	193	GLN	N-CA-CB	9.61	126.73	110.49
1	F	352	ASN	CA-CB-CG	-9.43	103.17	112.60
1	C	349	MET	N-CA-CB	-9.42	94.57	110.49
1	A	350	TRP	N-CA-C	9.42	125.29	110.32
1	A	34	ASN	CB-CA-C	-9.41	96.88	111.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	215	THR	N-CA-C	-9.31	95.82	108.38
1	G	475	ARG	N-CA-C	-9.13	91.35	110.80
1	B	341	LYS	N-CA-C	8.91	120.61	111.07
1	G	102	HIS	CA-CB-CG	8.82	122.62	113.80
1	C	49	ALA	N-CA-CB	-8.59	95.90	110.51
1	G	40	LEU	N-CA-CB	8.56	124.45	111.35
1	G	476	GLU	N-CA-C	-8.51	95.31	108.76
1	F	76	ILE	N-CA-C	-8.48	91.69	109.34
1	B	63	GLU	N-CA-C	-8.48	100.01	110.61
1	C	352	ASN	CA-CB-CG	8.42	121.02	112.60
1	E	257	ASP	N-CA-CB	8.41	123.62	110.84
1	D	386	ALA	N-CA-C	8.38	121.62	111.40
1	B	334	GLU	N-CA-C	8.36	121.14	111.11
1	C	60	THR	N-CA-C	-8.34	93.89	108.23
1	G	215	THR	N-CA-CB	8.30	124.35	111.24
1	B	256	ASN	N-CA-C	-8.30	96.20	109.39
1	C	48	SER	CB-CA-C	8.24	122.38	109.03
1	A	255	LEU	N-CA-C	8.22	123.55	111.96
1	D	60	THR	CA-CB-OG1	-8.13	97.41	109.60
1	E	45	THR	CB-CA-C	8.01	121.59	110.06
1	D	253	THR	CB-CA-C	7.96	121.62	110.16
1	F	474	SER	N-CA-C	-7.94	102.64	112.88
1	C	47	SER	N-CA-C	-7.91	98.32	110.10
1	G	257	ASP	N-CA-C	-7.88	94.02	110.80
1	G	130	GLU	N-CA-C	-7.83	99.46	110.50
1	G	256	ASN	N-CA-C	7.80	120.17	108.31
1	F	253	THR	CB-CA-C	7.62	121.27	109.84
1	A	131	PHE	CA-CB-CG	7.60	121.40	113.80
1	E	34	ASN	N-CA-C	7.59	121.87	111.39
1	E	341	LYS	N-CA-C	7.59	119.56	111.28
1	E	46	SER	N-CA-CB	-7.58	97.67	110.49
1	F	118	ASP	CA-CB-CG	7.58	120.18	112.60
1	C	473	ARG	N-CA-C	-7.57	103.11	111.36
1	D	350	TRP	N-CA-C	7.55	120.74	110.55
1	E	253	THR	CB-CA-C	7.55	121.67	109.90
1	A	130	GLU	N-CA-C	-7.43	100.02	110.50
1	A	47	SER	N-CA-C	-7.42	101.67	111.24
1	B	47	SER	N-CA-CB	-7.41	97.97	110.49
1	F	61	ASN	N-CA-CB	-7.40	98.82	110.22
1	E	380	ASN	N-CA-C	-7.36	99.56	110.46
1	E	253	THR	N-CA-C	-7.35	99.15	110.10
1	A	142	THR	N-CA-C	7.34	119.78	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	341	LYS	N-CA-C	7.33	119.91	111.11
1	G	41	ALA	N-CA-C	7.29	118.13	108.07
1	G	255	LEU	N-CA-C	-7.26	103.73	112.59
1	D	380	ASN	N-CA-C	-7.26	99.72	110.46
1	A	116	ILE	CA-C-N	-7.22	112.31	122.71
1	A	116	ILE	C-N-CA	-7.22	112.31	122.71
1	G	350	TRP	N-CA-C	7.21	121.18	110.52
1	G	65	THR	CB-CA-C	7.20	124.75	110.42
1	D	253	THR	N-CA-C	-7.14	99.32	109.96
1	C	380	ASN	N-CA-C	-7.14	99.89	110.46
1	F	253	THR	N-CA-C	-7.08	99.83	110.24
1	F	65	THR	N-CA-C	-7.04	104.82	113.41
1	B	131	PHE	N-CA-C	-7.04	105.05	112.93
1	A	350	TRP	N-CA-CB	-6.97	99.05	110.41
1	F	329	SER	N-CA-C	-6.97	104.29	114.39
1	F	472	ILE	N-CA-C	-6.97	102.34	110.21
1	G	41	ALA	CB-CA-C	-6.95	98.44	114.41
1	F	142	THR	N-CA-C	6.94	119.26	110.24
1	E	257	ASP	N-CA-C	-6.93	95.69	108.02
1	G	91	ARG	CA-CB-CG	-6.92	100.27	114.10
1	G	214	ASN	N-CA-C	-6.91	96.09	110.80
1	C	142	THR	N-CA-C	6.89	119.20	110.24
1	G	350	TRP	N-CA-CB	-6.86	99.49	110.46
1	B	142	THR	N-CA-C	6.85	119.40	110.43
1	C	215	THR	N-CA-C	-6.83	99.84	108.45
1	G	164	VAL	N-CA-C	-6.75	103.47	113.39
1	A	94	VAL	N-CA-C	-6.64	104.28	110.53
1	B	62	GLU	N-CA-C	6.58	117.75	108.00
1	E	142	THR	N-CA-C	6.53	119.22	110.35
1	D	386	ALA	CA-C-O	-6.52	113.58	120.55
1	C	48	SER	N-CA-C	-6.48	105.91	113.88
1	G	477	LEU	N-CA-CB	6.40	121.38	110.50
1	G	124	ILE	N-CA-C	-6.30	106.30	111.91
1	D	463	ASN	OD1-CG-ND2	-6.28	116.33	122.60
1	C	60	THR	N-CA-CB	-6.24	101.19	110.24
1	G	102	HIS	CB-CA-C	6.17	121.03	110.79
1	B	142	THR	N-CA-CB	-6.17	101.44	110.26
1	G	349	MET	CB-CA-C	-6.13	109.49	116.54
1	D	46	SER	CB-CA-C	-6.07	101.83	111.48
1	G	52	GLU	N-CA-C	-6.04	104.70	111.28
1	B	350	TRP	N-CA-C	6.02	118.78	110.35
1	C	349	MET	N-CA-C	-6.01	97.99	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	350	TRP	N-CA-CB	-6.00	101.32	110.45
1	D	61	ASN	N-CA-CB	-5.94	102.40	110.95
1	E	190	ARG	N-CA-C	-5.92	106.14	113.19
1	B	61	ASN	CA-C-O	-5.90	114.39	120.99
1	D	55	LYS	N-CA-C	-5.85	101.62	110.28
1	A	352	ASN	CA-CB-CG	5.84	118.44	112.60
1	D	142	THR	N-CA-C	5.83	118.28	110.35
1	D	385	ILE	N-CA-C	-5.83	99.95	108.11
1	C	47	SER	CB-CA-C	5.81	118.97	109.90
1	C	58	THR	N-CA-CB	-5.81	100.67	110.49
1	G	256	ASN	CB-CA-C	-5.76	109.92	116.54
1	B	130	GLU	CB-CA-C	-5.75	101.61	110.81
1	B	112	PRO	CB-CA-C	-5.72	104.54	111.46
1	C	256	ASN	N-CA-CB	5.68	120.08	110.49
1	D	34	ASN	N-CA-C	5.67	119.21	111.39
1	A	160	GLU	N-CA-C	-5.66	101.37	110.14
1	B	431	LEU	CA-C-O	-5.64	114.98	121.47
1	C	472	ILE	CB-CA-C	-5.61	104.79	111.97
1	C	255	LEU	N-CA-C	5.59	122.71	110.80
1	G	34	ASN	N-CA-C	5.59	119.11	111.39
1	G	140	PRO	CA-C-O	-5.57	117.09	121.38
1	A	329	SER	N-CA-C	-5.52	107.80	114.75
1	B	51	THR	N-CA-CB	5.50	120.01	110.44
1	E	108	MET	N-CA-C	5.47	118.25	110.10
1	E	76	ILE	N-CA-C	-5.44	107.67	112.90
1	G	105	ILE	N-CA-C	-5.43	101.96	109.46
1	D	46	SER	N-CA-C	5.43	119.20	112.47
1	D	118	ASP	CA-CB-CG	5.40	118.00	112.60
1	B	130	GLU	N-CA-C	5.39	117.58	111.11
1	F	218	ASP	CA-CB-CG	5.38	117.98	112.60
1	E	343	MET	CA-C-N	-5.38	117.68	122.47
1	E	343	MET	C-N-CA	-5.38	117.68	122.47
1	G	258	GLU	N-CA-CB	-5.36	105.77	113.65
1	E	84	THR	CA-CB-OG1	-5.33	101.60	109.60
1	F	64	LYS	CB-CA-C	-5.33	102.39	110.06
1	D	47	SER	N-CA-C	-5.28	100.56	108.96
1	B	329	SER	N-CA-C	-5.27	106.63	114.64
1	A	50	GLU	N-CA-C	-5.26	106.81	114.12
1	G	252	GLU	N-CA-C	5.26	117.86	109.65
1	B	259	VAL	N-CA-CB	5.24	117.28	110.57
1	F	355	GLU	CB-CG-CD	5.24	121.50	112.60
1	D	124	ILE	N-CA-C	-5.23	106.79	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	473	ARG	N-CA-C	-5.22	105.76	111.82
1	C	348	PRO	CB-CA-C	-5.21	102.95	111.56
1	G	259	VAL	N-CA-C	-5.20	105.43	110.42
1	G	305	VAL	CA-CB-CG1	5.19	119.22	110.40
1	B	431	LEU	N-CA-C	-5.17	102.83	110.48
1	C	48	SER	N-CA-CB	5.17	117.46	110.59
1	G	427	MET	CG-SD-CE	-5.16	89.56	100.90
1	D	255	LEU	CB-CA-C	-5.15	101.14	110.56
1	B	310	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	66	ILE	CB-CA-C	5.12	119.94	111.59
1	B	167	LYS	N-CA-C	-5.08	107.12	113.72
1	G	167	LYS	N-CA-C	-5.06	107.27	113.50
1	B	133	ILE	N-CA-C	5.06	117.12	109.12
1	D	472	ILE	N-CA-C	-5.04	107.48	111.81
1	A	384	MET	N-CA-C	5.03	116.84	109.24
1	D	471	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	115	LEU	CA-C-O	-5.01	115.37	121.88
1	B	349	MET	CB-CA-C	-5.01	109.33	116.34
1	G	331	TYR	CB-CA-C	5.00	119.41	111.51

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	ARG	Sidechain
1	A	179	ARG	Sidechain
1	A	228	ARG	Sidechain
1	A	234	ARG	Sidechain
1	A	248	ARG	Sidechain
1	A	249	ARG	Sidechain
1	A	326	ARG	Sidechain
1	A	409	ARG	Sidechain
1	A	421	ARG	Sidechain
1	B	111	ARG	Sidechain
1	B	179	ARG	Sidechain
1	B	190	ARG	Sidechain
1	B	248	ARG	Sidechain
1	B	306	ARG	Sidechain
1	B	326	ARG	Sidechain
1	B	421	ARG	Sidechain
1	B	473	ARG	Sidechain
1	C	111	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	248	ARG	Sidechain
1	C	421	ARG	Sidechain
1	C	429	ARG	Sidechain
1	C	473	ARG	Sidechain
1	C	91	ARG	Sidechain
1	D	107	SER	Mainchain
1	D	111	ARG	Sidechain
1	D	248	ARG	Sidechain
1	D	249	ARG	Sidechain
1	D	28	ARG	Sidechain
1	D	306	ARG	Sidechain
1	D	421	ARG	Sidechain
1	D	473	ARG	Sidechain
1	E	111	ARG	Sidechain
1	E	190	ARG	Sidechain
1	E	228	ARG	Sidechain
1	E	249	ARG	Sidechain
1	E	28	ARG	Sidechain
1	E	306	ARG	Sidechain
1	E	409	ARG	Sidechain
1	E	421	ARG	Sidechain
1	E	473	ARG	Sidechain
1	E	95	ARG	Sidechain
1	F	111	ARG	Sidechain
1	F	190	ARG	Sidechain
1	F	228	ARG	Sidechain
1	F	248	ARG	Sidechain
1	F	421	ARG	Sidechain
1	F	475	ARG	Sidechain
1	F	95	ARG	Sidechain
1	G	111	ARG	Sidechain
1	G	228	ARG	Sidechain
1	G	248	ARG	Sidechain
1	G	249	ARG	Sidechain
1	G	326	ARG	Sidechain
1	G	421	ARG	Sidechain
1	G	473	ARG	Sidechain
1	G	475	ARG	Sidechain
1	G	91	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3600	0	3690	161	1
1	B	3633	0	3723	131	1
1	C	3640	0	3730	155	0
1	D	3640	0	3729	135	0
1	E	3633	0	3723	171	0
1	F	3633	0	3722	126	0
1	G	3640	0	3729	195	0
2	A	36	0	21	1	0
2	B	36	0	20	3	0
2	C	36	0	20	15	0
2	D	36	0	20	5	0
2	E	36	0	20	10	0
2	F	36	0	20	4	0
2	G	36	0	20	5	0
3	A	14	0	0	2	0
3	B	14	0	0	1	0
3	C	14	0	0	1	0
3	D	14	0	0	1	0
3	F	14	0	0	1	0
All	All	25741	0	26187	1084	1

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 21.

All (1084) 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)
2:G:501:U2F:O4'	2:G:501:U2F:C4'	1.67	1.30
2:E:501:U2F:O4'	2:E:501:U2F:C4'	1.65	1.28
2:B:501:U2F:O4'	2:B:501:U2F:C4'	1.66	1.28
2:F:501:U2F:C4'	2:F:501:U2F:O4'	1.66	1.25
2:C:501:U2F:C4'	2:C:501:U2F:O4'	1.65	1.23
1:A:57:THR:CG2	1:A:68:ILE:HD13	1.70	1.21
2:D:501:U2F:O4'	2:D:501:U2F:C4'	1.66	1.19
1:A:115:LEU:CD2	1:A:128:ALA:HB2	1.74	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD12	1:A:68:ILE:HD12	1.30	1.12
1:G:10:ILE:H	1:G:39:ILE:HG22	0.99	1.12
1:G:10:ILE:HG13	1:G:39:ILE:HG21	1.32	1.11
1:E:176:LYS:HZ3	1:E:403:GLU:CG	1.63	1.10
1:E:176:LYS:NZ	1:E:403:GLU:HG2	1.67	1.09
1:A:429:ARG:HH11	1:A:433:GLN:CD	1.59	1.09
1:A:115:LEU:HD23	1:A:128:ALA:HB2	1.35	1.07
1:A:57:THR:HG23	1:A:68:ILE:HD13	1.29	1.06
1:G:10:ILE:H	1:G:39:ILE:CG2	1.70	1.05
1:A:122:THR:CG2	1:A:204:GLU:OE1	2.08	1.02
1:B:239:VAL:HG13	1:B:240:PRO:HD2	1.43	1.01
1:E:176:LYS:HZ3	1:E:403:GLU:HG2	1.17	1.01
1:A:429:ARG:NH1	1:A:433:GLN:NE2	2.12	0.97
1:B:239:VAL:CG1	1:B:240:PRO:HD2	1.95	0.96
1:A:10:ILE:HG23	1:A:116:ILE:HG21	1.46	0.94
1:E:12:SER:HB2	1:E:22:VAL:HG21	1.49	0.94
1:G:258:GLU:HG3	1:G:261:GLN:HB2	1.50	0.94
1:A:122:THR:HG23	1:A:204:GLU:OE1	1.66	0.93
1:A:429:ARG:NH1	1:A:433:GLN:CD	2.26	0.93
1:D:372:ASN:HB2	2:D:501:U2F:O1A	1.67	0.92
1:G:10:ILE:N	1:G:39:ILE:HG22	1.84	0.92
1:A:429:ARG:NH1	1:A:433:GLN:HE22	1.66	0.91
1:E:176:LYS:NZ	1:E:403:GLU:CG	2.28	0.91
1:F:351:ALA:O	2:F:501:U2F:H8'	1.71	0.90
1:A:231:GLU:O	1:A:235:LEU:HD23	1.71	0.90
1:B:81:ASN:O	1:B:84:THR:HG22	1.72	0.89
1:D:117:VAL:HG13	1:D:121:CYS:HB2	1.51	0.89
1:E:19:LEU:O	1:E:22:VAL:HG22	1.70	0.89
1:G:13:SER:HB3	1:G:14:PRO:HD2	1.52	0.88
1:A:57:THR:CG2	1:A:68:ILE:CD1	2.51	0.88
1:C:117:VAL:HG13	1:C:121:CYS:HB2	1.54	0.88
1:A:7:HIS:O	1:A:112:PRO:O	1.91	0.88
1:A:57:THR:HG23	1:A:68:ILE:CD1	2.03	0.88
1:E:183:VAL:CG1	1:E:187:LEU:HB2	2.02	0.88
1:C:146:LEU:HD13	1:C:213:ILE:HD11	1.54	0.88
1:D:55:LYS:O	1:D:56:LYS:HG2	1.75	0.87
1:G:183:VAL:O	1:G:394:LYS:HD2	1.74	0.87
1:E:413:LEU:HD23	1:E:414:PRO:HD2	1.58	0.86
1:G:153:GLN:OE1	1:G:203:LYS:HD3	1.75	0.86
1:E:413:LEU:HD23	1:E:414:PRO:CD	2.06	0.85
1:B:292:TRP:CD1	1:B:421:ARG:HH21	1.93	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ILE:HG12	1:A:116:ILE:HD13	1.57	0.85
1:C:332:LEU:HD13	1:C:336:PHE:HB3	1.58	0.85
1:A:115:LEU:HD22	1:A:128:ALA:HB2	1.56	0.85
1:A:105:ILE:O	1:A:108:MET:HG2	1.77	0.85
1:F:239:VAL:HG22	1:F:240:PRO:HD2	1.59	0.84
1:C:185:ASP:HA	1:C:188:LEU:HD13	1.59	0.84
1:F:364:GLY:HA3	1:F:432:MET:HE1	1.60	0.84
1:G:38:THR:CG2	1:G:69:ILE:HD11	2.08	0.84
1:D:103:SER:O	1:D:106:ALA:O	1.95	0.83
1:A:122:THR:HG21	1:A:204:GLU:OE1	1.76	0.83
1:A:42:ILE:HD11	1:A:101:ILE:HD11	1.59	0.83
1:A:141:THR:HG22	1:A:371:TRP:CB	2.09	0.83
1:A:299:GLN:NE2	1:A:433:GLN:NE2	2.27	0.83
1:G:234:ARG:HD2	1:G:234:ARG:O	1.79	0.83
1:A:210:GLY:C	1:A:211:ILE:HD12	2.03	0.82
1:E:5:GLN:HG3	1:E:34:ASN:O	1.78	0.82
1:F:266:GLN:OE1	1:F:300:LYS:HE2	1.80	0.82
1:C:348:PRO:O	1:C:349:MET:HE2	1.80	0.82
1:E:119:ILE:HD11	1:E:120:PHE:CE1	2.14	0.82
1:D:157:LYS:HA	1:D:157:LYS:CE	2.10	0.82
1:G:249:ARG:NH2	2:G:501:U2F:O2'	2.12	0.81
1:E:251:VAL:HG23	1:E:355:GLU:HG3	1.61	0.81
1:A:81:ASN:OD1	1:A:84:THR:OG1	1.98	0.80
1:F:141:THR:HG22	1:F:371:TRP:CB	2.10	0.80
1:C:146:LEU:CD1	1:C:213:ILE:HD11	2.12	0.80
1:E:409:ARG:HG2	1:E:409:ARG:HH11	1.44	0.80
1:G:476:GLU:O	1:G:477:LEU:HD23	1.81	0.80
1:G:38:THR:HG22	1:G:69:ILE:CD1	2.11	0.80
1:A:65:THR:HG23	1:A:66:ILE:HG12	1.62	0.79
1:B:80:ILE:HB	1:B:84:THR:HG21	1.65	0.79
1:A:14:PRO:O	1:A:50:GLU:OE2	2.00	0.79
1:A:299:GLN:NE2	1:A:433:GLN:HE21	1.80	0.79
1:C:290:LEU:O	1:C:294:LEU:HD12	1.82	0.79
1:G:255:LEU:HD23	1:G:261:GLN:HG2	1.62	0.79
1:G:38:THR:HG22	1:G:69:ILE:HD12	1.65	0.79
1:D:307:PRO:HD3	1:D:349:MET:HE1	1.63	0.78
1:B:290:LEU:O	1:B:294:LEU:HD12	1.83	0.78
1:D:257:ASP:OD1	1:D:258:GLU:N	2.16	0.78
1:D:332:LEU:C	1:D:333:PRO:O	2.18	0.78
1:D:290:LEU:O	1:D:294:LEU:HD12	1.83	0.78
1:C:68:ILE:C	1:C:69:ILE:HD12	2.10	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:LYS:HE3	1:G:285:LYS:HA	1.64	0.77
1:G:37:ILE:HG22	1:G:39:ILE:HG23	1.66	0.77
1:B:244:ILE:HG23	1:B:465:ILE:HD11	1.65	0.77
1:A:290:LEU:O	1:A:294:LEU:HD12	1.84	0.77
1:C:305:VAL:O	1:C:348:PRO:O	2.03	0.77
1:A:103:SER:O	1:A:106:ALA:O	2.04	0.76
1:A:429:ARG:NH1	1:A:433:GLN:OE1	1.95	0.76
3:C:502:T83:OAC	3:C:502:T83:CAA	2.33	0.76
1:G:274:VAL:HG13	1:G:366:LEU:HD23	1.66	0.76
1:G:38:THR:HG21	1:G:69:ILE:HD11	1.67	0.76
1:G:285:LYS:HA	1:G:285:LYS:CE	2.15	0.76
1:B:377:SER:O	1:B:382:VAL:HG22	1.86	0.76
1:F:29:LEU:HB2	1:F:37:ILE:HD11	1.67	0.75
1:F:150:ILE:HD13	1:F:237:LEU:HD23	1.68	0.75
1:A:10:ILE:HG23	1:A:116:ILE:CG2	2.16	0.75
1:A:7:HIS:ND1	1:A:112:PRO:HA	2.01	0.75
1:A:377:SER:O	1:A:382:VAL:HG22	1.86	0.75
1:D:290:LEU:HD22	1:D:303:TRP:CZ2	2.22	0.75
1:D:392:GLU:HG2	1:D:396:ASN:ND2	2.02	0.75
1:E:373:SER:OG	2:E:501:U2F:H5'2	1.87	0.75
1:A:299:GLN:HE22	1:A:433:GLN:HE21	1.33	0.74
1:G:38:THR:CG2	1:G:69:ILE:CD1	2.64	0.74
1:D:150:ILE:HD13	1:D:237:LEU:HD23	1.69	0.74
1:D:430:ILE:HA	1:D:434:THR:HG23	1.69	0.74
1:C:56:LYS:O	1:C:57:THR:C	2.27	0.74
1:E:148:LEU:HD23	1:E:172:ILE:HD11	1.70	0.74
1:F:341:LYS:HE2	1:F:342:ASP:OD1	1.87	0.74
2:C:501:U2F:PB	2:C:501:U2F:H4'	2.27	0.73
1:G:292:TRP:O	1:G:296:LEU:HD22	1.87	0.73
1:B:295:GLU:OE1	1:B:339:ARG:HD2	1.88	0.73
1:B:142:THR:HG21	1:B:399:MET:HE1	1.69	0.73
2:E:501:U2F:O1A	2:E:501:U2F:H4'	1.84	0.73
1:G:80:ILE:HD11	1:G:92:LEU:HD11	1.69	0.73
1:G:285:LYS:HE3	1:G:288:THR:OG1	1.88	0.73
1:A:150:ILE:HD13	1:A:237:LEU:HD23	1.70	0.73
1:A:304:VAL:HG13	1:A:349:MET:O	1.89	0.73
1:G:40:LEU:HG	1:G:41:ALA:H	1.54	0.73
1:A:57:THR:HG21	1:A:68:ILE:HD13	1.68	0.72
1:C:213:ILE:HG22	1:C:215:THR:HG22	1.69	0.72
1:G:162:GLU:OE2	1:G:165:GLU:CD	2.32	0.72
1:B:71:VAL:HG13	1:B:100:LYS:HG2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:183:VAL:HG11	1:E:187:LEU:HB2	1.70	0.72
1:F:143:ALA:N	1:F:213:ILE:HD11	2.03	0.72
1:E:57:THR:O	1:E:59:LEU:HD12	1.90	0.72
1:G:118:ASP:OD1	1:G:119:ILE:HG22	1.89	0.72
3:D:502:T83:OAC	3:D:502:T83:CAA	2.37	0.71
1:F:36:LYS:HD3	1:F:65:THR:HA	1.72	0.71
1:E:203:LYS:O	1:E:206:THR:HG22	1.90	0.71
1:G:76:ILE:HB	1:G:96:GLU:OE1	1.90	0.71
1:B:251:VAL:HG13	1:B:355:GLU:HG3	1.72	0.71
1:D:203:LYS:O	1:D:206:THR:HG22	1.90	0.71
1:E:431:LEU:O	1:E:431:LEU:HD23	1.91	0.71
3:F:502:T83:OAC	3:F:502:T83:CAA	2.38	0.71
1:B:292:TRP:O	1:B:296:LEU:HD12	1.90	0.71
1:F:141:THR:HG22	1:F:371:TRP:HB2	1.72	0.71
1:G:10:ILE:CG1	1:G:39:ILE:HG21	2.16	0.71
1:A:203:LYS:O	1:A:206:THR:HG22	1.91	0.71
1:B:137:THR:HG21	1:B:205:TYR:HD1	1.56	0.71
1:A:141:THR:HG22	1:A:371:TRP:HB2	1.73	0.70
1:A:115:LEU:HD23	1:A:128:ALA:CB	2.19	0.70
1:C:429:ARG:NH2	1:D:260:ILE:CG2	2.54	0.70
1:G:278:SER:O	1:G:306:ARG:NH1	2.23	0.70
1:C:352:ASN:HB2	1:C:355:GLU:OE1	1.92	0.70
1:F:203:LYS:O	1:F:206:THR:HG22	1.92	0.70
1:G:203:LYS:O	1:G:206:THR:HG22	1.92	0.70
1:G:466:CYS:O	1:G:470:LYS:HG2	1.92	0.70
3:B:502:T83:OAC	3:B:502:T83:CAA	2.39	0.70
1:B:185:ASP:HA	1:B:188:LEU:HD23	1.73	0.69
1:C:88:THR:O	1:C:92:LEU:HD13	1.91	0.69
1:D:117:VAL:HG11	1:D:121:CYS:O	1.92	0.69
1:D:292:TRP:O	1:D:296:LEU:HD12	1.92	0.69
1:A:406:VAL:CG2	1:A:444:ALA:HB2	2.22	0.69
1:C:56:LYS:C	1:C:57:THR:O	2.27	0.69
1:E:413:LEU:CD2	1:E:415:THR:H	2.04	0.69
1:G:89:GLN:O	1:G:93:LEU:HG	1.93	0.69
1:G:153:GLN:OE1	1:G:203:LYS:CD	2.39	0.69
1:F:248:ARG:HD2	1:F:379:THR:HG21	1.73	0.69
1:G:185:ASP:HA	1:G:188:LEU:HD23	1.73	0.69
1:A:38:THR:HG22	1:A:67:GLU:HB3	1.74	0.69
1:A:141:THR:HG21	1:A:392:GLU:OE2	1.93	0.69
1:F:137:THR:HG21	1:F:205:TYR:HD1	1.58	0.69
1:F:166:LEU:HD13	1:F:168:GLU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:GLU:HG3	1:C:331:TYR:CD1	2.28	0.69
1:D:332:LEU:O	1:D:333:PRO:C	2.35	0.69
1:E:413:LEU:HD23	1:E:414:PRO:N	2.08	0.69
1:E:87:PHE:HB3	1:E:194:GLN:HG2	1.74	0.68
1:E:215:THR:OG1	1:E:219:LEU:HD23	1.93	0.68
1:B:50:GLU:O	1:B:50:GLU:HG2	1.93	0.68
1:D:430:ILE:HA	1:D:434:THR:CG2	2.23	0.68
1:C:48:SER:O	1:C:52:GLU:OE2	2.12	0.68
1:F:141:THR:HG21	1:F:392:GLU:OE2	1.93	0.68
1:E:185:ASP:HA	1:E:188:LEU:HD23	1.74	0.68
1:A:8:VAL:HG12	1:A:114:ALA:HB3	1.76	0.68
1:G:244:ILE:HG22	1:G:244:ILE:O	1.90	0.68
1:G:256:ASN:HB2	1:G:260:ILE:HD13	1.74	0.68
1:A:352:ASN:HB3	1:A:355:GLU:OE1	1.92	0.67
1:C:244:ILE:HG23	1:C:465:ILE:HD11	1.76	0.67
1:A:10:ILE:HG12	1:A:116:ILE:CD1	2.25	0.67
1:C:185:ASP:HA	1:C:188:LEU:CD1	2.23	0.67
1:C:117:VAL:HG11	1:C:121:CYS:O	1.94	0.67
1:G:40:LEU:HG	1:G:41:ALA:N	2.08	0.67
1:G:273:PHE:HE2	1:G:353:GLN:HG3	1.59	0.67
1:A:115:LEU:HD21	1:A:124:ILE:HG22	1.76	0.67
1:F:239:VAL:HG22	1:F:240:PRO:CD	2.23	0.67
1:D:157:LYS:HA	1:D:157:LYS:HE2	1.73	0.67
1:E:466:CYS:O	1:E:470:LYS:HG2	1.93	0.66
1:G:76:ILE:HG13	1:G:78:HIS:H	1.59	0.66
1:G:90:LEU:O	1:G:94:VAL:HG13	1.96	0.66
1:E:14:PRO:O	1:E:50:GLU:OE1	2.13	0.66
1:D:273:PHE:HE2	1:D:353:GLN:HG3	1.61	0.66
1:F:137:THR:HG21	1:F:205:TYR:CD1	2.31	0.66
1:G:87:PHE:HE1	1:G:91:ARG:NH2	1.94	0.66
1:E:146:LEU:HD13	1:E:146:LEU:C	2.21	0.66
1:A:54:LEU:CD1	1:A:68:ILE:HD12	2.19	0.66
1:G:352:ASN:HB3	1:G:355:GLU:OE1	1.96	0.66
1:C:297:SER:HB2	1:C:428:VAL:CG2	2.25	0.65
1:B:352:ASN:HB3	1:B:355:GLU:OE1	1.95	0.65
1:D:281:THR:HG23	1:D:306:ARG:NH1	2.11	0.65
1:E:88:THR:HG21	1:E:193:GLN:HG2	1.76	0.65
1:F:76:ILE:HG13	1:F:93:LEU:HD22	1.78	0.65
1:E:19:LEU:O	1:E:22:VAL:CG2	2.43	0.65
1:E:372:ASN:HB2	2:E:501:U2F:O1A	1.96	0.65
1:B:137:THR:HG21	1:B:205:TYR:CD1	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:HG22	1:A:371:TRP:HB3	1.78	0.65
1:C:115:LEU:CD1	1:C:133:ILE:HG21	2.27	0.65
1:F:328:MET:HA	1:F:331:TYR:CE1	2.32	0.65
1:C:244:ILE:HG22	1:C:244:ILE:O	1.97	0.65
1:E:183:VAL:HG12	1:E:187:LEU:HB2	1.79	0.65
1:D:429:ARG:O	1:D:433:GLN:HG2	1.95	0.65
1:F:219:LEU:HD12	1:F:220:GLU:HG3	1.79	0.65
1:B:112:PRO:HG2	1:B:133:ILE:HD13	1.79	0.64
1:C:466:CYS:O	1:C:470:LYS:HG3	1.96	0.64
1:D:392:GLU:HG2	1:D:396:ASN:HD21	1.58	0.64
1:E:438:LYS:N	1:E:438:LYS:HD2	2.12	0.64
1:F:222:GLU:N	1:F:222:GLU:OE1	2.29	0.64
1:A:463:ASN:O	1:A:467:GLU:OE1	2.15	0.64
1:B:244:ILE:HG22	1:B:244:ILE:O	1.95	0.64
1:F:101:ILE:HD13	1:F:124:ILE:HD11	1.80	0.64
1:G:423:GLU:O	1:G:427:MET:HG3	1.98	0.64
1:E:176:LYS:NZ	1:E:403:GLU:HG3	2.10	0.64
1:D:176:LYS:NZ	1:D:403:GLU:HG3	2.13	0.63
1:A:273:PHE:HE2	1:A:353:GLN:HG3	1.62	0.63
1:B:239:VAL:HG12	1:B:240:PRO:HD2	1.80	0.63
1:E:352:ASN:HB3	1:E:355:GLU:OE1	1.98	0.63
1:C:94:VAL:HG23	1:C:123:GLN:NE2	2.13	0.63
1:E:213:ILE:HG23	1:E:215:THR:HG22	1.80	0.63
1:D:176:LYS:HZ2	1:D:403:GLU:HG3	1.62	0.63
1:B:111:ARG:HH22	1:G:255:LEU:HD21	1.64	0.63
1:D:332:LEU:O	1:D:333:PRO:O	2.17	0.63
1:E:468:LEU:C	1:E:468:LEU:HD13	2.24	0.63
1:C:332:LEU:HD13	1:C:336:PHE:CB	2.29	0.62
1:G:304:VAL:HG13	1:G:349:MET:O	2.00	0.62
1:A:119:ILE:HG13	1:A:201:LEU:HD11	1.82	0.62
1:C:239:VAL:HG22	1:C:240:PRO:HD2	1.80	0.62
1:E:383:PRO:HG2	1:E:431:LEU:HD21	1.81	0.62
1:F:272:LEU:HD13	1:F:432:MET:HE3	1.80	0.62
1:A:117:VAL:HG23	1:A:137:THR:HG23	1.80	0.62
2:C:501:U2F:H4'	2:C:501:U2F:O1B	2.00	0.62
1:D:352:ASN:HB3	1:D:355:GLU:OE1	1.98	0.62
1:E:176:LYS:HZ2	1:E:403:GLU:HG2	1.60	0.62
1:G:57:THR:O	1:G:57:THR:HG22	2.00	0.62
1:D:157:LYS:HE2	1:D:157:LYS:CA	2.30	0.62
1:A:299:GLN:HE21	1:A:433:GLN:NE2	1.98	0.62
1:E:272:LEU:HD22	1:E:428:VAL:HG13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:196:GLU:O	1:G:200:LYS:HG3	2.00	0.62
1:D:468:LEU:HD13	1:D:468:LEU:C	2.25	0.61
1:E:413:LEU:HD22	1:E:415:THR:HB	1.81	0.61
1:A:126:PRO:O	1:A:129:GLU:HG3	1.99	0.61
1:G:139:HIS:ND1	1:G:146:LEU:HB2	2.15	0.61
1:B:286:GLN:OE1	1:B:419:VAL:HG23	2.00	0.61
1:D:259:VAL:HG13	1:D:345:LEU:HD23	1.82	0.61
1:G:277:GLY:HA3	1:G:368:HIS:CE1	2.36	0.61
1:B:353:GLN:NE2	1:B:376:GLU:OE1	2.34	0.61
1:E:251:VAL:CG2	1:E:355:GLU:HG3	2.30	0.61
1:G:255:LEU:HD23	1:G:261:GLN:CG	2.28	0.61
1:B:76:ILE:CD1	1:B:93:LEU:HD22	2.30	0.61
1:D:115:LEU:CD2	1:D:117:VAL:HG23	2.31	0.61
1:A:16:MET:SD	1:A:53:PHE:HD2	2.24	0.61
1:B:201:LEU:HD13	1:B:201:LEU:C	2.26	0.61
1:E:14:PRO:HG2	1:E:93:LEU:HD23	1.82	0.61
1:E:213:ILE:HG22	1:E:243:PRO:HA	1.82	0.61
1:E:413:LEU:HD13	1:E:416:LYS:HD3	1.83	0.61
1:G:108:MET:CE	1:G:112:PRO:HD3	2.31	0.61
1:G:109:THR:OG1	1:G:110:HIS:CD2	2.54	0.61
1:D:106:ALA:HA	1:D:111:ARG:HH12	1.64	0.60
1:E:201:LEU:HD13	1:E:201:LEU:C	2.26	0.60
1:E:248:ARG:HD3	1:E:379:THR:HG21	1.83	0.60
1:C:350:TRP:CZ2	2:C:501:U2F:H8'	2.36	0.60
1:D:19:LEU:HD23	1:D:19:LEU:C	2.26	0.60
1:B:464:SER:O	1:B:467:GLU:HG2	2.01	0.60
1:D:201:LEU:HD13	1:D:201:LEU:C	2.26	0.60
1:G:122:THR:OG1	1:G:204:GLU:OE1	2.13	0.60
1:E:57:THR:O	1:E:59:LEU:CD1	2.49	0.60
1:A:105:ILE:C	1:A:108:MET:HG2	2.27	0.60
1:E:286:GLN:HE22	1:E:419:VAL:H	1.50	0.60
1:G:38:THR:HG23	1:G:67:GLU:HG3	1.82	0.60
1:A:277:GLY:O	1:A:306:ARG:NH2	2.34	0.60
1:C:76:ILE:CD1	1:C:93:LEU:HD22	2.31	0.60
1:C:297:SER:CB	1:C:428:VAL:HG21	2.30	0.60
2:E:501:U2F:O6'	2:E:501:U2F:C2'	2.48	0.60
1:F:141:THR:HG22	1:F:371:TRP:HB3	1.82	0.60
1:G:76:ILE:HG23	1:G:77:SER:H	1.67	0.60
1:A:115:LEU:C	1:A:116:ILE:HG13	2.27	0.60
1:C:466:CYS:HA	1:C:469:VAL:HG22	1.83	0.60
1:E:409:ARG:HH11	1:E:409:ARG:CG	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:166:LEU:CD1	1:F:168:GLU:H	2.15	0.60
1:G:286:GLN:HE22	1:G:419:VAL:H	1.50	0.60
1:D:117:VAL:HG11	1:D:121:CYS:C	2.27	0.59
2:C:501:U2F:H3'	2:C:501:U2F:O3A	2.02	0.59
1:B:10:ILE:CG2	1:B:22:VAL:HG13	2.33	0.59
1:B:142:THR:HG22	1:B:145:THR:HG23	1.83	0.59
1:C:117:VAL:HG11	1:C:121:CYS:C	2.27	0.59
1:E:183:VAL:HG11	1:E:187:LEU:CB	2.31	0.59
1:G:91:ARG:HG2	1:G:91:ARG:HH11	1.68	0.59
1:C:332:LEU:HD12	1:C:333:PRO:O	2.02	0.59
1:G:212:LEU:HD23	1:G:244:ILE:HD12	1.85	0.59
1:G:244:ILE:O	1:G:244:ILE:CG2	2.50	0.59
1:C:371:TRP:N	2:C:501:U2F:O4	2.27	0.59
1:D:7:HIS:HE1	1:D:108:MET:HE1	1.68	0.59
1:E:162:GLU:O	1:E:165:GLU:HG2	2.02	0.59
1:B:50:GLU:O	1:B:50:GLU:CG	2.49	0.59
1:C:251:VAL:HG13	1:C:355:GLU:HG3	1.85	0.59
1:D:19:LEU:HD23	1:D:19:LEU:O	2.02	0.59
1:A:16:MET:SD	1:A:50:GLU:CB	2.91	0.59
1:C:212:LEU:HD23	1:C:244:ILE:HD12	1.84	0.59
1:C:372:ASN:HB2	2:C:501:U2F:H1'	1.84	0.59
1:E:148:LEU:HD12	1:E:198:TYR:OH	2.03	0.59
1:F:286:GLN:HE22	1:F:419:VAL:H	1.49	0.59
1:B:239:VAL:CG1	1:B:240:PRO:CD	2.78	0.58
1:G:137:THR:HG23	1:G:208:PHE:CD2	2.38	0.58
1:G:373:SER:OG	2:G:501:U2F:O2A	2.20	0.58
1:E:328:MET:HA	1:E:331:TYR:CE1	2.39	0.58
1:D:326:ARG:HB3	1:D:330:GLU:OE2	2.03	0.58
1:A:148:LEU:HD12	1:A:198:TYR:OH	2.03	0.58
1:C:373:SER:OG	2:C:501:U2F:O2'	2.21	0.58
1:B:292:TRP:CD1	1:B:421:ARG:NH2	2.70	0.58
1:G:10:ILE:N	1:G:39:ILE:CG2	2.52	0.58
1:G:235:LEU:HA	1:G:238:LYS:NZ	2.19	0.58
1:A:406:VAL:HG23	1:A:444:ALA:HB2	1.86	0.58
1:E:263:LEU:HB3	1:E:359:HIS:ND1	2.19	0.58
3:A:502:T83:OAC	3:A:502:T83:CAA	2.51	0.58
1:D:115:LEU:HD21	1:D:117:VAL:HG23	1.86	0.58
1:C:213:ILE:CG2	1:C:215:THR:HG22	2.33	0.58
1:D:327:ASP:O	1:D:328:MET:C	2.47	0.58
1:G:117:VAL:HG23	1:G:137:THR:HG22	1.85	0.58
1:D:148:LEU:HD12	1:D:198:TYR:OH	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:10:ILE:CG2	1:F:22:VAL:HG13	2.34	0.58
1:G:4:SER:OG	1:G:36:LYS:NZ	2.31	0.58
1:A:429:ARG:CZ	1:A:433:GLN:HE22	2.16	0.57
1:E:399:MET:HG2	1:E:404:LEU:CD2	2.34	0.57
1:A:211:ILE:HD12	1:A:211:ILE:N	2.19	0.57
1:D:249:ARG:NH2	1:D:354:VAL:HG23	2.19	0.57
1:F:263:LEU:HB3	1:F:359:HIS:ND1	2.19	0.57
1:G:412:VAL:HG11	1:G:417:LYS:HD3	1.86	0.57
1:C:263:LEU:HB3	1:C:359:HIS:ND1	2.20	0.57
1:F:217:GLU:HG2	1:F:224:ILE:HD12	1.85	0.57
1:A:10:ILE:HA	1:A:116:ILE:HB	1.87	0.57
1:C:286:GLN:HE22	1:C:419:VAL:H	1.52	0.57
1:C:297:SER:CB	1:C:428:VAL:CG2	2.82	0.57
1:F:290:LEU:HD13	1:F:303:TRP:CZ2	2.40	0.57
1:B:76:ILE:HD11	1:B:93:LEU:HD22	1.87	0.57
1:D:259:VAL:HG13	1:D:345:LEU:CD2	2.35	0.57
1:F:148:LEU:HD12	1:F:198:TYR:OH	2.03	0.57
1:F:172:ILE:HD12	1:F:172:ILE:H	1.70	0.57
1:A:113:ASP:HB3	1:A:476:GLU:OE2	2.05	0.57
1:A:105:ILE:O	1:A:108:MET:CG	2.52	0.57
1:A:117:VAL:HG21	1:A:122:THR:HA	1.86	0.57
1:G:475:ARG:O	1:G:476:GLU:CD	2.48	0.57
1:B:61:ASN:O	1:B:62:GLU:HG2	2.05	0.57
1:B:244:ILE:O	1:B:244:ILE:CG2	2.53	0.57
1:C:141:THR:OG1	1:C:142:THR:N	2.38	0.57
1:F:98:LEU:HA	1:F:101:ILE:HD12	1.85	0.57
1:F:239:VAL:CG2	1:F:240:PRO:HD2	2.32	0.56
1:B:89:GLN:O	1:B:93:LEU:HD23	2.05	0.56
1:C:327:ASP:O	1:C:330:GLU:HG2	2.05	0.56
1:D:286:GLN:HE22	1:D:419:VAL:H	1.50	0.56
1:D:290:LEU:HD23	1:D:294:LEU:CD1	2.35	0.56
1:D:299:GLN:NE2	1:D:433:GLN:OE1	2.38	0.56
1:E:246:PRO:HD2	1:E:455:LEU:HD11	1.88	0.56
1:G:148:LEU:HD22	1:G:178:LEU:CD2	2.35	0.56
1:A:16:MET:CE	1:A:53:PHE:CD2	2.88	0.56
1:C:307:PRO:HD3	1:C:349:MET:HE1	1.87	0.56
1:C:139:HIS:CE1	1:C:141:THR:HG23	2.41	0.56
1:C:350:TRP:HA	1:C:350:TRP:CE3	2.41	0.56
1:G:106:ALA:HB2	1:G:131:PHE:CZ	2.40	0.56
1:B:244:ILE:CG2	1:B:465:ILE:HD11	2.36	0.56
1:F:239:VAL:CG2	1:F:240:PRO:CD	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASP:C	1:B:239:VAL:HG11	2.31	0.56
1:C:424:ILE:O	1:C:428:VAL:HG13	2.06	0.56
1:D:78:HIS:CE1	1:D:79:LEU:HD21	2.40	0.56
1:D:277:GLY:HA3	1:D:368:HIS:CE1	2.41	0.56
1:G:13:SER:HA	1:G:42:ILE:HD12	1.87	0.56
1:G:268:ASN:O	1:G:269:GLU:HG2	2.05	0.56
1:B:336:PHE:HA	1:B:339:ARG:NH1	2.20	0.56
1:G:40:LEU:CG	1:G:41:ALA:H	2.17	0.56
1:D:263:LEU:HB3	1:D:359:HIS:ND1	2.21	0.56
1:E:95:ARG:HA	1:E:98:LEU:HD23	1.88	0.56
1:E:373:SER:OG	2:E:501:U2F:C5'	2.54	0.56
1:D:304:VAL:HG13	1:D:349:MET:O	2.06	0.56
1:G:72:PRO:O	1:G:100:LYS:CE	2.54	0.56
1:D:22:VAL:HG12	1:D:39:ILE:CD1	2.36	0.55
1:A:34:ASN:CG	1:A:34:ASN:O	2.44	0.55
1:A:54:LEU:O	1:A:58:THR:HG23	2.06	0.55
1:E:13:SER:HB3	1:E:14:PRO:CD	2.37	0.55
1:B:115:LEU:CD2	1:B:117:VAL:HG12	2.37	0.55
1:F:249:ARG:HH21	1:F:354:VAL:HG22	1.72	0.55
1:G:48:SER:O	1:G:50:GLU:HG3	2.06	0.55
1:E:431:LEU:HD23	1:E:431:LEU:C	2.32	0.55
1:B:148:LEU:HD22	1:B:178:LEU:CD2	2.36	0.55
1:C:244:ILE:O	1:C:244:ILE:CG2	2.55	0.55
1:D:53:PHE:O	1:D:57:THR:OG1	2.24	0.55
1:G:153:GLN:O	1:G:157:LYS:HD3	2.06	0.55
1:D:10:ILE:CG2	1:D:22:VAL:HG13	2.37	0.55
1:F:353:GLN:OE1	2:F:501:U2F:H2'	2.07	0.55
1:B:5:GLN:HG3	1:B:34:ASN:O	2.07	0.55
1:C:78:HIS:CE1	1:C:79:LEU:HG	2.42	0.55
1:C:230:ASN:OD1	1:C:232:LYS:N	2.36	0.55
1:E:119:ILE:HD11	1:E:120:PHE:CD1	2.41	0.55
1:F:89:GLN:O	1:F:93:LEU:HD23	2.06	0.55
1:F:251:VAL:HG13	1:F:355:GLU:HG2	1.88	0.55
1:A:476:GLU:OE1	1:A:476:GLU:HA	2.06	0.54
2:E:501:U2F:O6'	2:E:501:U2F:C3'	2.56	0.54
1:F:95:ARG:HA	1:F:98:LEU:HD23	1.90	0.54
1:F:266:GLN:CD	1:F:300:LYS:HE2	2.33	0.54
1:C:89:GLN:O	1:C:93:LEU:HD23	2.07	0.54
1:F:292:TRP:CZ3	1:F:295:GLU:OE1	2.60	0.54
1:G:72:PRO:O	1:G:100:LYS:HE3	2.07	0.54
1:A:377:SER:HB2	1:A:382:VAL:HG23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ASN:HA	1:B:375:VAL:HG22	1.90	0.54
1:B:377:SER:HB2	1:B:382:VAL:HG23	1.90	0.54
1:C:76:ILE:HD11	1:C:93:LEU:HD22	1.89	0.54
1:D:236:LEU:HD12	1:D:236:LEU:N	2.23	0.54
1:F:286:GLN:NE2	1:F:419:VAL:HG23	2.22	0.54
1:G:86:ILE:HA	1:G:89:GLN:HB2	1.90	0.54
1:A:328:MET:HA	1:A:331:TYR:CZ	2.43	0.54
1:B:273:PHE:HE2	1:B:353:GLN:HG3	1.72	0.54
1:C:29:LEU:HB2	1:C:37:ILE:HD11	1.89	0.54
1:F:197:GLU:HA	1:F:197:GLU:OE1	2.07	0.54
1:A:10:ILE:CG2	1:A:22:VAL:HG13	2.38	0.54
1:G:87:PHE:CE1	1:G:91:ARG:CZ	2.91	0.54
1:B:244:ILE:HG23	1:B:465:ILE:CD1	2.35	0.54
1:C:408:ILE:HD12	1:C:430:ILE:HD11	1.88	0.54
1:D:95:ARG:HA	1:D:98:LEU:HD23	1.89	0.54
1:E:468:LEU:C	1:E:468:LEU:CD1	2.81	0.54
1:F:29:LEU:CB	1:F:37:ILE:HD11	2.36	0.54
1:C:248:ARG:HH21	1:C:354:VAL:CG1	2.21	0.54
1:G:118:ASP:OD1	1:G:119:ILE:N	2.38	0.54
1:D:246:PRO:HB2	1:D:375:VAL:HG13	1.90	0.53
1:D:468:LEU:C	1:D:468:LEU:CD1	2.81	0.53
1:D:7:HIS:CE1	1:D:108:MET:HE1	2.44	0.53
1:E:119:ILE:CD1	1:E:120:PHE:CD1	2.92	0.53
1:E:273:PHE:HE2	1:E:353:GLN:HG3	1.74	0.53
1:A:277:GLY:HA3	1:A:368:HIS:CE1	2.43	0.53
1:B:193:GLN:HE21	1:B:197:GLU:HG2	1.74	0.53
1:C:142:THR:OG1	1:C:145:THR:HG23	2.08	0.53
1:E:119:ILE:CG2	1:E:139:HIS:HA	2.38	0.53
1:F:59:LEU:O	1:F:59:LEU:HG	2.08	0.53
1:F:236:LEU:HD12	1:F:236:LEU:N	2.22	0.53
1:A:112:PRO:O	1:A:113:ASP:HB2	2.08	0.53
1:B:95:ARG:HA	1:B:98:LEU:HD23	1.90	0.53
1:G:122:THR:HG21	1:G:201:LEU:HD11	1.91	0.53
1:A:249:ARG:NH2	1:A:354:VAL:HG23	2.24	0.53
1:C:10:ILE:CG2	1:C:22:VAL:HG13	2.38	0.53
1:E:148:LEU:CD2	1:E:172:ILE:HD11	2.38	0.53
1:E:430:ILE:O	1:E:434:THR:OG1	2.24	0.53
1:F:166:LEU:HD12	1:F:168:GLU:O	2.09	0.53
1:F:263:LEU:HB3	1:F:359:HIS:HD1	1.74	0.53
1:F:273:PHE:HE2	1:F:353:GLN:HG3	1.74	0.53
1:G:475:ARG:O	1:G:476:GLU:CG	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ILE:O	1:B:428:VAL:HG12	2.08	0.53
1:B:442:GLU:O	1:B:446:LYS:CD	2.57	0.53
1:C:117:VAL:CG1	1:C:121:CYS:C	2.82	0.53
1:C:429:ARG:NH2	1:D:260:ILE:HG23	2.24	0.53
1:F:105:ILE:HA	1:F:108:MET:HE3	1.90	0.53
1:A:43:THR:HG22	1:A:71:VAL:O	2.09	0.53
1:C:95:ARG:HA	1:C:98:LEU:HD23	1.90	0.53
1:D:117:VAL:CG1	1:D:121:CYS:C	2.81	0.53
1:E:246:PRO:HB2	1:E:375:VAL:HG13	1.89	0.53
1:F:359:HIS:HD2	1:G:433:GLN:O	1.92	0.53
1:G:106:ALA:HB2	1:G:131:PHE:CE2	2.44	0.53
1:G:236:LEU:N	1:G:236:LEU:HD12	2.23	0.53
1:A:95:ARG:HA	1:A:98:LEU:HD23	1.90	0.52
1:B:111:ARG:HH12	1:G:255:LEU:HD22	1.74	0.52
1:F:430:ILE:O	1:F:434:THR:OG1	2.26	0.52
1:G:268:ASN:C	1:G:269:GLU:HG2	2.34	0.52
1:C:337:LEU:HD12	1:C:337:LEU:H	1.74	0.52
1:F:5:GLN:HG3	1:F:34:ASN:O	2.09	0.52
1:G:274:VAL:CG1	1:G:366:LEU:HD23	2.37	0.52
1:E:277:GLY:HA3	1:E:368:HIS:CE1	2.44	0.52
1:G:463:ASN:HA	1:G:466:CYS:SG	2.50	0.52
1:C:69:ILE:HD12	1:C:69:ILE:N	2.24	0.52
1:F:142:THR:OG1	1:F:145:THR:HG23	2.09	0.52
1:F:449:LYS:O	1:F:453:ASN:OD1	2.28	0.52
1:A:16:MET:SD	1:A:50:GLU:HB2	2.49	0.52
1:B:336:PHE:HA	1:B:339:ARG:HH11	1.74	0.52
1:D:353:GLN:OE1	2:D:501:U2F:H2'	2.09	0.52
1:F:9:ALA:O	1:F:115:LEU:HD12	2.10	0.52
1:G:463:ASN:O	1:G:466:CYS:SG	2.54	0.52
1:E:143:ALA:HA	1:E:213:ILE:HD11	1.91	0.52
1:E:399:MET:HG2	1:E:404:LEU:HD21	1.91	0.52
1:E:119:ILE:HG22	1:E:139:HIS:HA	1.92	0.52
1:A:142:THR:OG1	1:A:145:THR:HG23	2.09	0.52
1:E:90:LEU:HD22	1:E:120:PHE:CE2	2.45	0.52
1:B:442:GLU:O	1:B:446:LYS:HD3	2.10	0.52
1:C:126:PRO:HA	1:C:129:GLU:HG3	1.92	0.52
1:D:142:THR:HG23	1:D:145:THR:HG23	1.92	0.52
1:E:94:VAL:HG23	1:E:123:GLN:OE1	2.09	0.52
1:E:176:LYS:HZ3	1:E:403:GLU:HG3	1.61	0.52
1:A:148:LEU:HD13	1:A:148:LEU:C	2.35	0.52
1:B:212:LEU:HD23	1:B:244:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:ILE:HD12	1:G:127:ILE:HG23	1.91	0.52
1:A:248:ARG:HD3	1:A:379:THR:HG21	1.92	0.51
1:B:22:VAL:HG12	1:B:39:ILE:HD12	1.90	0.51
1:D:290:LEU:CD2	1:D:294:LEU:HD11	2.40	0.51
1:E:183:VAL:O	1:E:394:LYS:HE2	2.10	0.51
1:F:217:GLU:HA	1:F:224:ILE:CD1	2.40	0.51
1:B:383:PRO:HB2	1:B:431:LEU:HD11	1.91	0.51
1:E:292:TRP:O	1:E:296:LEU:HD22	2.10	0.51
1:C:423:GLU:O	1:C:427:MET:HG3	2.11	0.51
1:D:146:LEU:HD23	1:D:213:ILE:HD11	1.93	0.51
1:E:148:LEU:HD13	1:E:148:LEU:C	2.35	0.51
1:G:182:ASP:O	1:G:394:LYS:HG3	2.11	0.51
1:B:292:TRP:CG	1:B:421:ARG:HH21	2.26	0.51
1:F:10:ILE:HG21	1:F:22:VAL:HG13	1.92	0.51
1:F:148:LEU:HD13	1:F:148:LEU:C	2.35	0.51
1:D:10:ILE:HG21	1:D:22:VAL:HG13	1.93	0.51
1:D:55:LYS:C	1:D:56:LYS:HG2	2.35	0.51
1:D:101:ILE:HD13	1:D:124:ILE:HD11	1.91	0.51
1:D:148:LEU:C	1:D:148:LEU:HD13	2.35	0.51
1:A:401:THR:HG21	1:A:409:ARG:HD3	1.92	0.51
1:C:21:PRO:O	1:C:24:VAL:HG22	2.10	0.51
1:G:337:LEU:HD12	1:G:337:LEU:H	1.74	0.51
1:E:20:ILE:HG21	1:E:249:ARG:HD3	1.91	0.51
1:E:14:PRO:HB3	1:E:44:THR:HG22	1.93	0.51
1:E:468:LEU:HD13	1:E:468:LEU:O	2.10	0.51
1:G:137:THR:CG2	1:G:208:PHE:CE2	2.93	0.51
1:A:14:PRO:O	1:A:50:GLU:CD	2.53	0.51
1:D:327:ASP:O	1:D:330:GLU:HG2	2.11	0.51
1:G:466:CYS:O	1:G:469:VAL:HG12	2.10	0.51
1:E:290:LEU:HD22	1:E:303:TRP:CZ2	2.46	0.51
1:A:193:GLN:O	1:A:196:GLU:HG2	2.11	0.50
1:G:290:LEU:HD22	1:G:303:TRP:CZ2	2.47	0.50
2:C:501:U2F:H5'1	2:C:501:U2F:H9'	1.94	0.50
1:C:328:MET:HA	1:C:331:TYR:CZ	2.47	0.50
1:D:55:LYS:O	1:D:56:LYS:CG	2.55	0.50
1:D:257:ASP:OD2	1:D:260:ILE:HG12	2.10	0.50
1:E:402:GLU:HB2	1:E:403:GLU:OE1	2.11	0.50
1:F:290:LEU:C	1:F:290:LEU:CD2	2.85	0.50
1:E:413:LEU:HD22	1:E:415:THR:N	2.26	0.50
1:G:50:GLU:O	1:G:53:PHE:HB2	2.11	0.50
1:G:122:THR:CG2	1:G:201:LEU:HD11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HG21	1:B:22:VAL:HG13	1.94	0.50
1:C:42:ILE:HA	1:C:71:VAL:HG13	1.92	0.50
1:C:435:LYS:HZ1	1:D:382:VAL:HG22	1.77	0.50
1:G:86:ILE:O	1:G:87:PHE:C	2.55	0.50
1:G:366:LEU:HD11	1:G:387:TRP:CE3	2.47	0.50
1:A:246:PRO:HB2	1:A:375:VAL:HG13	1.93	0.50
1:D:118:ASP:OD1	1:D:119:ILE:N	2.45	0.50
1:F:290:LEU:C	1:F:290:LEU:HD23	2.37	0.50
1:G:290:LEU:HD22	1:G:303:TRP:CH2	2.47	0.50
1:B:255:LEU:HD22	1:B:257:ASP:HB2	1.94	0.50
1:C:297:SER:HB2	1:C:428:VAL:HG22	1.93	0.50
1:C:350:TRP:HZ2	2:C:501:U2F:O7'	1.95	0.50
1:E:292:TRP:C	1:E:296:LEU:HD22	2.37	0.50
1:F:172:ILE:HD12	1:F:172:ILE:N	2.27	0.50
1:D:301:PHE:CE1	1:D:344:GLY:HA3	2.47	0.50
1:A:121:CYS:HB3	1:A:124:ILE:HD12	1.93	0.50
1:D:141:THR:OG1	1:D:142:THR:N	2.45	0.50
1:G:252:GLU:HG2	1:G:355:GLU:OE2	2.12	0.50
1:B:52:GLU:HA	1:B:55:LYS:HE2	1.93	0.49
1:C:114:ALA:C	1:C:115:LEU:HD12	2.37	0.49
1:E:290:LEU:HD22	1:E:303:TRP:CH2	2.47	0.49
1:F:29:LEU:HB2	1:F:37:ILE:CD1	2.39	0.49
1:F:109:THR:HG23	1:F:110:HIS:N	2.27	0.49
1:B:73:SER:OG	1:B:74:VAL:N	2.44	0.49
1:D:22:VAL:HG12	1:D:39:ILE:HD12	1.95	0.49
1:G:8:VAL:O	1:G:37:ILE:HG23	2.13	0.49
1:G:141:THR:CG2	1:G:142:THR:H	2.25	0.49
1:G:290:LEU:HD23	1:G:290:LEU:C	2.37	0.49
1:B:44:THR:HG21	1:B:47:SER:HB3	1.95	0.49
1:C:44:THR:HA	1:C:73:SER:OG	2.12	0.49
1:D:98:LEU:HD11	1:D:123:GLN:O	2.12	0.49
1:A:231:GLU:HG3	1:A:232:LYS:N	2.27	0.49
1:D:118:ASP:OD1	1:D:119:ILE:HG22	2.11	0.49
1:D:468:LEU:HD13	1:D:468:LEU:O	2.10	0.49
1:E:119:ILE:HG23	1:E:140:PRO:HD3	1.94	0.49
1:F:98:LEU:HD11	1:F:123:GLN:O	2.12	0.49
1:G:246:PRO:HB2	1:G:375:VAL:HG13	1.94	0.49
1:G:249:ARG:HH21	2:G:501:U2F:C2'	2.25	0.49
1:A:337:LEU:HD12	1:A:337:LEU:H	1.75	0.49
1:C:101:ILE:HG22	1:C:105:ILE:HD11	1.95	0.49
1:A:136:TYR:OH	1:A:471:ASP:OD1	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:115:LEU:HD13	1:C:133:ILE:CG2	2.43	0.49
1:D:284:THR:HG22	1:D:310:ASP:OD1	2.11	0.49
1:E:413:LEU:CD2	1:E:415:THR:HB	2.43	0.49
1:G:42:ILE:HA	1:G:71:VAL:O	2.13	0.49
1:E:337:LEU:H	1:E:337:LEU:HD12	1.78	0.49
1:A:470:LYS:HD3	1:A:470:LYS:C	2.37	0.49
1:B:251:VAL:HG22	1:B:354:VAL:HG22	1.94	0.49
1:F:261:GLN:HE21	1:G:298:GLN:HE21	1.61	0.49
1:G:372:ASN:HB2	2:G:501:U2F:O5'	2.12	0.49
1:A:124:ILE:HG23	1:A:127:ILE:HD11	1.94	0.49
1:G:335:GLY:O	1:G:338:THR:HG22	2.13	0.49
1:B:98:LEU:HA	1:B:101:ILE:HD12	1.94	0.49
1:B:248:ARG:HD3	1:B:379:THR:HG21	1.95	0.49
1:B:385:ILE:HG23	1:B:427:MET:HE2	1.94	0.49
1:C:251:VAL:CG1	1:C:355:GLU:HG3	2.43	0.49
1:F:16:MET:HE1	1:F:53:PHE:CD2	2.48	0.49
1:F:118:ASP:OD1	1:F:119:ILE:N	2.46	0.49
1:C:247:LEU:HD23	1:C:455:LEU:HD11	1.93	0.48
1:E:244:ILE:CG2	1:E:465:ILE:HD11	2.43	0.48
1:E:290:LEU:C	1:E:290:LEU:HD23	2.37	0.48
1:E:413:LEU:HD22	1:E:415:THR:H	1.76	0.48
1:G:87:PHE:CE1	1:G:91:ARG:NH2	2.78	0.48
1:D:157:LYS:CE	1:D:157:LYS:CA	2.85	0.48
1:G:146:LEU:C	1:G:146:LEU:CD1	2.86	0.48
1:B:301:PHE:CE1	1:B:344:GLY:HA3	2.47	0.48
1:B:327:ASP:O	1:B:328:MET:HB2	2.13	0.48
1:F:341:LYS:HG3	1:F:342:ASP:N	2.28	0.48
1:G:95:ARG:O	1:G:98:LEU:HD22	2.14	0.48
1:A:20:ILE:O	1:A:24:VAL:HG13	2.13	0.48
1:A:115:LEU:HG	1:A:116:ILE:H	1.77	0.48
1:B:295:GLU:CD	1:B:339:ARG:HD2	2.38	0.48
1:G:162:GLU:OE1	1:G:162:GLU:N	2.29	0.48
1:G:354:VAL:HG23	1:G:355:GLU:CD	2.38	0.48
1:A:124:ILE:O	1:A:125:LEU:C	2.56	0.48
1:A:377:SER:HB2	1:A:382:VAL:CG2	2.43	0.48
1:C:413:LEU:HB2	1:C:416:LYS:HE2	1.94	0.48
1:F:76:ILE:HD11	1:F:93:LEU:HA	1.95	0.48
1:G:292:TRP:C	1:G:296:LEU:HD22	2.39	0.48
1:A:10:ILE:HG21	1:A:22:VAL:HG13	1.96	0.48
1:A:376:GLU:O	1:A:380:ASN:ND2	2.43	0.48
1:E:401:THR:HG21	1:E:409:ARG:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:HA	1:A:168:GLU:OE1	2.14	0.48
1:B:292:TRP:O	1:B:296:LEU:CD1	2.60	0.48
1:E:21:PRO:O	1:E:24:VAL:HG22	2.14	0.48
1:E:34:ASN:O	1:E:34:ASN:CG	2.56	0.48
1:E:119:ILE:HD11	1:E:120:PHE:CZ	2.48	0.48
1:A:14:PRO:HA	1:A:42:ILE:O	2.14	0.48
1:B:332:LEU:N	1:B:332:LEU:HD12	2.29	0.48
1:F:468:LEU:C	1:F:468:LEU:HD23	2.38	0.48
2:B:501:U2F:H9'	2:B:501:U2F:H5'1	1.95	0.48
1:C:5:GLN:NE2	1:C:36:LYS:HB2	2.29	0.48
1:C:86:ILE:O	1:C:90:LEU:HD23	2.14	0.48
1:A:45:THR:OG1	1:A:73:SER:N	2.47	0.48
1:C:430:ILE:O	1:C:434:THR:OG1	2.26	0.48
1:E:59:LEU:HD12	1:E:59:LEU:N	2.29	0.48
1:F:251:VAL:HG13	1:F:355:GLU:CG	2.43	0.47
1:G:62:GLU:H	1:G:62:GLU:HG2	1.38	0.47
1:A:454:ALA:O	1:A:455:LEU:HB2	2.15	0.47
1:C:246:PRO:HB2	1:C:375:VAL:HG13	1.95	0.47
1:A:16:MET:SD	1:A:50:GLU:HB3	2.54	0.47
1:B:105:ILE:O	1:B:111:ARG:NH1	2.47	0.47
1:C:117:VAL:HG13	1:C:121:CYS:CB	2.36	0.47
1:E:20:ILE:HD13	1:E:249:ARG:HD3	1.97	0.47
1:A:117:VAL:CG2	1:A:137:THR:HG23	2.44	0.47
1:B:242:PHE:CE2	1:B:467:GLU:HG3	2.49	0.47
1:G:121:CYS:HB3	1:G:124:ILE:HD12	1.95	0.47
1:G:146:LEU:HD13	1:G:146:LEU:O	2.14	0.47
1:A:105:ILE:HA	1:A:108:MET:HG2	1.96	0.47
1:A:115:LEU:O	1:A:116:ILE:HG13	2.14	0.47
1:E:8:VAL:HG22	1:E:114:ALA:HB3	1.97	0.47
1:E:234:ARG:HH12	1:E:237:LEU:HD12	1.79	0.47
2:E:501:U2F:O6'	2:E:501:U2F:H2'	2.14	0.47
1:F:26:GLY:HA2	1:F:37:ILE:HD13	1.96	0.47
1:G:473:ARG:HE	1:G:473:ARG:HB3	1.57	0.47
1:B:115:LEU:HD21	1:B:117:VAL:HG12	1.95	0.47
1:B:326:ARG:HB3	1:B:331:TYR:HE1	1.80	0.47
2:C:501:U2F:O1B	2:C:501:U2F:H5	2.15	0.47
1:E:141:THR:OG1	1:E:142:THR:N	2.39	0.47
1:C:141:THR:HA	1:C:371:TRP:CD1	2.50	0.47
1:C:392:GLU:OE2	2:C:501:U2F:H4	2.15	0.47
1:D:290:LEU:HD22	1:D:303:TRP:CH2	2.49	0.47
1:D:337:LEU:HD12	1:D:337:LEU:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:203:LYS:O	1:F:206:THR:CG2	2.62	0.47
1:F:387:TRP:CH2	1:F:419:VAL:HG21	2.50	0.47
1:G:94:VAL:O	1:G:98:LEU:HD13	2.14	0.47
1:B:74:VAL:HG22	1:B:75:ASP:N	2.29	0.47
1:E:33:HIS:CE1	1:E:465:ILE:HG21	2.50	0.47
1:F:213:ILE:HD13	1:F:215:THR:HG22	1.96	0.47
1:G:156:ASP:O	1:G:190:ARG:NH2	2.47	0.47
1:A:16:MET:SD	1:A:53:PHE:CD2	3.06	0.47
1:B:20:ILE:O	1:B:24:VAL:HG13	2.14	0.47
1:D:156:ASP:OD1	1:D:190:ARG:NH2	2.48	0.47
1:E:5:GLN:HE21	1:E:34:ASN:C	2.22	0.46
1:F:212:LEU:HD23	1:F:244:ILE:HD13	1.97	0.46
1:F:263:LEU:HB3	1:F:359:HIS:CE1	2.51	0.46
1:F:263:LEU:CB	1:F:359:HIS:HD1	2.28	0.46
1:F:424:ILE:O	1:F:428:VAL:HG12	2.15	0.46
1:A:426:GLY:O	1:A:427:MET:C	2.58	0.46
1:E:112:PRO:HB2	1:E:133:ILE:HD13	1.97	0.46
1:E:466:CYS:HA	1:E:469:VAL:HG12	1.97	0.46
2:E:501:U2F:O2A	2:E:501:U2F:O5	2.32	0.46
1:G:20:ILE:HD13	1:G:249:ARG:HD3	1.97	0.46
1:A:81:ASN:O	1:A:82:SER:C	2.57	0.46
1:A:141:THR:HA	1:A:371:TRP:CD1	2.50	0.46
1:B:125:LEU:HB3	1:B:126:PRO:HD3	1.97	0.46
1:E:203:LYS:O	1:E:206:THR:CG2	2.62	0.46
1:F:392:GLU:OE2	2:F:501:U2F:O3	2.33	0.46
1:E:263:LEU:HB3	1:E:359:HIS:CE1	2.50	0.46
1:G:13:SER:HB3	1:G:14:PRO:CD	2.34	0.46
1:G:102:HIS:O	1:G:105:ILE:HG12	2.15	0.46
1:B:433:GLN:O	1:B:438:LYS:HE2	2.15	0.46
1:C:277:GLY:HA3	1:C:368:HIS:CE1	2.51	0.46
1:G:38:THR:HG23	1:G:67:GLU:CG	2.46	0.46
1:G:57:THR:O	1:G:58:THR:C	2.58	0.46
1:A:156:ASP:OD1	1:A:190:ARG:NH2	2.49	0.46
1:F:166:LEU:HD13	1:F:167:LYS:N	2.31	0.46
1:A:465:ILE:H	1:A:465:ILE:HG13	1.52	0.46
1:B:377:SER:HB2	1:B:382:VAL:CG2	2.45	0.46
1:C:263:LEU:HB3	1:C:359:HIS:CE1	2.51	0.46
1:C:456:SER:O	1:C:457:ASP:C	2.58	0.46
1:D:7:HIS:ND1	1:D:112:PRO:HA	2.31	0.46
1:D:292:TRP:O	1:D:296:LEU:CD1	2.61	0.46
1:A:130:GLU:C	1:A:132:ASN:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:ALA:O	1:C:50:GLU:C	2.59	0.46
1:D:396:ASN:O	1:D:400:LEU:HG	2.15	0.46
1:F:468:LEU:HD23	1:F:468:LEU:O	2.16	0.46
1:A:382:VAL:HG23	1:A:382:VAL:O	2.16	0.46
1:B:115:LEU:C	1:B:115:LEU:HD23	2.41	0.46
1:B:194:GLN:H	1:B:194:GLN:HG3	1.58	0.46
1:C:468:LEU:O	1:C:472:ILE:HG12	2.16	0.46
1:D:19:LEU:C	1:D:19:LEU:CD2	2.89	0.46
1:G:12:SER:HB3	1:G:41:ALA:HB2	1.98	0.46
1:G:248:ARG:HD3	1:G:379:THR:HG21	1.97	0.46
1:A:48:SER:HB2	1:A:51:THR:CG2	2.46	0.46
1:A:65:THR:O	1:A:66:ILE:C	2.59	0.46
1:A:94:VAL:O	1:A:95:ARG:C	2.57	0.46
1:C:427:MET:HA	1:C:430:ILE:HG12	1.98	0.46
1:C:429:ARG:NH2	1:D:264:ASP:OD2	2.49	0.46
1:D:369:CYS:SG	1:D:386:ALA:O	2.64	0.46
1:E:76:ILE:O	1:E:77:SER:C	2.58	0.46
1:C:7:HIS:ND1	1:C:112:PRO:HA	2.30	0.45
1:D:203:LYS:O	1:D:206:THR:CG2	2.62	0.45
1:D:372:ASN:CB	2:D:501:U2F:O1A	2.51	0.45
1:G:257:ASP:O	1:G:258:GLU:HB3	2.15	0.45
1:C:156:ASP:OD1	1:C:190:ARG:NH2	2.49	0.45
2:D:501:U2F:H9'	2:D:501:U2F:H5'2	1.98	0.45
1:E:244:ILE:CG2	1:E:244:ILE:O	2.64	0.45
1:E:299:GLN:NE2	1:E:433:GLN:HG3	2.32	0.45
1:G:6:LEU:HB3	1:G:35:ILE:HG23	1.99	0.45
1:G:95:ARG:HD2	1:G:95:ARG:HA	1.83	0.45
2:A:501:U2F:O6	3:A:502:T83:OAC	2.33	0.45
1:B:237:LEU:HD22	1:B:239:VAL:H	1.81	0.45
1:F:143:ALA:CA	1:F:213:ILE:CD1	2.95	0.45
1:A:203:LYS:O	1:A:206:THR:CG2	2.62	0.45
1:C:173:PRO:HB2	1:C:233:LEU:HG	1.98	0.45
1:D:249:ARG:CZ	1:D:354:VAL:HG23	2.47	0.45
1:F:141:THR:HA	1:F:371:TRP:CD1	2.51	0.45
1:F:143:ALA:HA	1:F:213:ILE:HD12	1.98	0.45
1:C:13:SER:OG	1:C:18:HIS:CB	2.65	0.45
1:C:46:SER:O	1:C:47:SER:C	2.58	0.45
1:E:53:PHE:CE1	1:E:57:THR:HG21	2.52	0.45
1:E:59:LEU:CD1	1:E:59:LEU:N	2.79	0.45
1:E:125:LEU:HB3	1:E:126:PRO:HD3	1.98	0.45
1:F:137:THR:HG23	1:F:211:ILE:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:424:ILE:O	1:G:428:VAL:HG12	2.16	0.45
1:A:290:LEU:HD23	1:A:303:TRP:CZ2	2.51	0.45
1:F:246:PRO:HB2	1:F:375:VAL:HG13	1.97	0.45
1:B:105:ILE:HA	1:B:108:MET:CE	2.46	0.45
2:C:501:U2F:H3'	2:C:501:U2F:PA	2.57	0.45
1:D:263:LEU:HB3	1:D:359:HIS:CE1	2.52	0.45
1:C:476:GLU:HA	1:C:476:GLU:OE1	2.17	0.45
1:D:78:HIS:CE1	1:D:79:LEU:CD2	2.99	0.45
1:G:203:LYS:O	1:G:206:THR:CG2	2.63	0.45
1:B:100:LYS:O	1:B:101:ILE:C	2.60	0.45
1:B:290:LEU:HD23	1:B:303:TRP:CZ2	2.51	0.45
1:D:114:ALA:CB	1:D:472:ILE:HD13	2.47	0.45
1:D:176:LYS:HD2	1:D:403:GLU:OE2	2.17	0.45
1:E:305:VAL:HG13	1:E:328:MET:HE2	1.98	0.45
2:E:501:U2F:O6'	2:E:501:U2F:H3'	2.17	0.45
1:G:40:LEU:HD13	1:G:68:ILE:HG12	1.98	0.45
1:G:130:GLU:C	1:G:132:ASN:H	2.24	0.45
1:B:239:VAL:HG12	1:B:240:PRO:CD	2.46	0.45
1:C:124:ILE:O	1:C:125:LEU:C	2.59	0.45
1:E:246:PRO:HD2	1:E:455:LEU:CD1	2.46	0.45
1:G:91:ARG:O	1:G:95:ARG:N	2.34	0.45
1:A:328:MET:HA	1:A:331:TYR:CE2	2.52	0.44
1:D:117:VAL:HG13	1:D:121:CYS:CB	2.36	0.44
1:G:48:SER:C	1:G:50:GLU:H	2.25	0.44
1:A:249:ARG:CZ	1:A:354:VAL:HG23	2.47	0.44
1:B:137:THR:HG23	1:B:211:ILE:HG23	1.99	0.44
1:C:376:GLU:O	1:C:380:ASN:ND2	2.42	0.44
1:D:115:LEU:HD23	1:D:115:LEU:C	2.42	0.44
1:E:353:GLN:NE2	1:E:376:GLU:OE1	2.35	0.44
1:F:217:GLU:HA	1:F:224:ILE:HD12	1.98	0.44
1:F:253:THR:HG22	1:G:425:GLN:HE22	1.82	0.44
1:G:7:HIS:HA	1:G:36:LYS:O	2.18	0.44
1:G:44:THR:C	1:G:46:SER:H	2.24	0.44
1:A:43:THR:CG2	1:A:72:PRO:HA	2.47	0.44
1:A:48:SER:HB2	1:A:51:THR:HG21	1.98	0.44
1:B:76:ILE:HD11	1:B:93:LEU:CD2	2.47	0.44
1:F:286:GLN:CD	1:F:419:VAL:HG23	2.42	0.44
1:F:468:LEU:C	1:F:468:LEU:CD2	2.91	0.44
1:C:94:VAL:CG2	1:C:123:GLN:HE21	2.30	0.44
1:E:95:ARG:CA	1:E:98:LEU:HD23	2.48	0.44
1:A:43:THR:OG1	1:A:44:THR:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.83	0.44
1:C:10:ILE:HG21	1:C:22:VAL:HG13	1.98	0.44
1:C:69:ILE:N	1:C:69:ILE:CD1	2.80	0.44
1:E:296:LEU:N	1:E:296:LEU:HD13	2.32	0.44
1:F:86:ILE:O	1:F:90:LEU:HD23	2.16	0.44
1:F:253:THR:HG21	1:G:425:GLN:NE2	2.33	0.44
1:G:153:GLN:CD	1:G:203:LYS:HD3	2.39	0.44
1:A:115:LEU:HG	1:A:116:ILE:N	2.32	0.44
1:B:44:THR:CG2	1:B:47:SER:HB3	2.48	0.44
1:B:366:LEU:C	1:B:366:LEU:HD23	2.43	0.44
1:C:94:VAL:CG2	1:C:123:GLN:NE2	2.79	0.44
1:C:258:GLU:OE2	1:E:132:ASN:ND2	2.51	0.44
1:C:429:ARG:HH22	1:D:260:ILE:HG22	1.81	0.44
1:D:106:ALA:HA	1:D:111:ARG:NH1	2.30	0.44
1:G:57:THR:O	1:G:57:THR:CG2	2.65	0.44
1:B:72:PRO:HD2	1:B:100:LYS:HD3	1.98	0.44
1:C:221:PRO:HG2	1:C:222:GLU:OE1	2.18	0.44
1:D:100:LYS:HD2	1:D:100:LYS:HA	1.71	0.44
1:E:145:THR:HG21	1:E:392:GLU:HG3	2.00	0.44
1:G:117:VAL:CG2	1:G:137:THR:HG22	2.47	0.44
1:C:244:ILE:HG23	1:C:465:ILE:CD1	2.47	0.44
1:D:124:ILE:O	1:D:125:LEU:C	2.61	0.44
1:E:14:PRO:HA	1:E:42:ILE:O	2.18	0.44
1:E:201:LEU:HD13	1:E:201:LEU:O	2.18	0.44
1:F:105:ILE:HA	1:F:108:MET:CE	2.48	0.44
1:G:141:THR:CG2	1:G:142:THR:N	2.81	0.44
1:A:105:ILE:CA	1:A:108:MET:HG2	2.48	0.44
1:D:366:LEU:HD23	1:D:366:LEU:C	2.43	0.44
1:E:343:MET:HB3	1:E:343:MET:HE3	1.47	0.44
1:E:413:LEU:HD23	1:E:413:LEU:C	2.43	0.44
1:G:5:GLN:OE1	1:G:35:ILE:HA	2.18	0.44
1:G:33:HIS:CE1	1:G:465:ILE:HD13	2.53	0.44
1:G:475:ARG:O	1:G:476:GLU:HG3	2.17	0.44
1:A:263:LEU:HB3	1:A:359:HIS:CD2	2.52	0.43
1:C:408:ILE:CD1	1:C:430:ILE:HG13	2.48	0.43
1:D:95:ARG:CA	1:D:98:LEU:HD23	2.48	0.43
1:E:19:LEU:HD22	1:E:50:GLU:HG3	2.00	0.43
1:E:383:PRO:CG	1:E:431:LEU:HD21	2.46	0.43
1:G:7:HIS:HD1	1:G:112:PRO:HA	1.83	0.43
1:A:211:ILE:N	1:A:211:ILE:CD1	2.82	0.43
1:C:130:GLU:C	1:C:132:ASN:H	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:PRO:HG2	1:D:93:LEU:HD12	2.00	0.43
1:D:151:TYR:HD2	1:D:155:PHE:CE2	2.36	0.43
1:E:234:ARG:NH1	1:E:237:LEU:HD12	2.32	0.43
1:E:399:MET:O	1:E:404:LEU:HD22	2.18	0.43
1:A:366:LEU:C	1:A:366:LEU:HD23	2.43	0.43
1:A:409:ARG:HB2	1:A:410:PRO:HD2	2.01	0.43
1:C:38:THR:HG23	1:C:69:ILE:HD13	2.00	0.43
1:C:366:LEU:C	1:C:366:LEU:HD23	2.43	0.43
1:F:143:ALA:CA	1:F:213:ILE:HD11	2.47	0.43
1:F:209:ASP:C	1:F:239:VAL:HG21	2.43	0.43
1:G:301:PHE:CZ	1:G:344:GLY:HA3	2.53	0.43
1:A:95:ARG:CA	1:A:98:LEU:HD23	2.49	0.43
1:B:7:HIS:ND1	1:B:112:PRO:HA	2.33	0.43
1:C:104:THR:O	1:C:108:MET:HG2	2.19	0.43
1:C:409:ARG:HB2	1:C:410:PRO:HD2	2.01	0.43
1:E:366:LEU:C	1:E:366:LEU:HD23	2.43	0.43
1:F:349:MET:HB3	1:F:350:TRP:H	1.70	0.43
1:G:137:THR:CG2	1:G:208:PHE:CD2	3.01	0.43
1:B:52:GLU:O	1:B:56:LYS:HG2	2.19	0.43
1:B:286:GLN:CD	1:B:419:VAL:HG23	2.42	0.43
1:B:382:VAL:HG23	1:B:382:VAL:O	2.18	0.43
1:C:95:ARG:CA	1:C:98:LEU:HD23	2.49	0.43
1:C:146:LEU:C	1:C:146:LEU:HD23	2.43	0.43
1:E:27:ASN:HA	1:E:66:ILE:HD11	2.01	0.43
1:E:119:ILE:C	1:E:119:ILE:HD12	2.43	0.43
1:E:295:GLU:HB3	1:E:296:LEU:HD13	2.01	0.43
1:F:366:LEU:C	1:F:366:LEU:HD23	2.43	0.43
1:G:88:THR:OG1	1:G:89:GLN:N	2.52	0.43
1:G:432:MET:HE3	1:G:432:MET:HB3	1.86	0.43
1:A:151:TYR:HD2	1:A:155:PHE:CE2	2.37	0.43
1:C:42:ILE:HA	1:C:71:VAL:CG1	2.49	0.43
1:D:10:ILE:HB	1:D:39:ILE:HD13	1.99	0.43
1:D:213:ILE:HG22	1:D:215:THR:HG22	2.00	0.43
1:E:130:GLU:C	1:E:132:ASN:H	2.25	0.43
1:G:404:LEU:N	1:G:404:LEU:HD12	2.33	0.43
1:A:33:HIS:O	1:A:35:ILE:HG13	2.18	0.43
1:A:35:ILE:HD11	1:A:469:VAL:CG1	2.49	0.43
1:B:10:ILE:HG22	1:B:22:VAL:HG13	1.99	0.43
1:B:64:LYS:C	1:B:66:ILE:H	2.25	0.43
1:C:94:VAL:HG23	1:C:123:GLN:HE21	1.82	0.43
1:C:229:TYR:CD2	1:F:430:ILE:HD11	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:MET:HA	1:C:331:TYR:CE2	2.54	0.43
1:D:201:LEU:HD13	1:D:201:LEU:O	2.18	0.43
1:E:413:LEU:HD13	1:E:416:LYS:CE	2.48	0.43
1:F:301:PHE:CZ	1:F:344:GLY:HA3	2.53	0.43
1:G:72:PRO:O	1:G:100:LYS:HD3	2.18	0.43
1:G:90:LEU:HD13	1:G:120:PHE:CZ	2.54	0.43
1:G:139:HIS:HE1	1:G:146:LEU:N	2.16	0.43
1:B:106:ALA:O	1:B:111:ARG:NH1	2.50	0.43
1:B:301:PHE:CZ	1:B:344:GLY:HA3	2.53	0.43
1:D:27:ASN:HA	1:D:66:ILE:HD11	2.00	0.43
1:D:409:ARG:HB2	1:D:410:PRO:HD2	2.01	0.43
1:F:58:THR:O	1:F:59:LEU:HB3	2.18	0.43
1:G:153:GLN:CD	1:G:203:LYS:CD	2.92	0.43
1:A:301:PHE:CZ	1:A:344:GLY:HA3	2.54	0.43
1:B:145:THR:HG21	1:B:392:GLU:HG3	2.01	0.43
1:C:61:ASN:OD1	1:C:61:ASN:O	2.37	0.43
1:C:80:ILE:HG22	1:C:84:THR:HG21	2.01	0.43
1:G:139:HIS:CE1	1:G:146:LEU:HB2	2.54	0.43
1:B:115:LEU:CD2	1:B:117:VAL:CG1	2.97	0.43
1:C:44:THR:HA	1:C:73:SER:HG	1.84	0.43
1:C:59:LEU:HD22	1:C:59:LEU:H	1.84	0.43
1:C:125:LEU:HB3	1:C:126:PRO:HD3	2.01	0.43
1:C:259:VAL:HG23	1:C:260:ILE:N	2.33	0.43
1:C:429:ARG:NH2	1:D:260:ILE:HG22	2.30	0.43
1:A:466:CYS:HA	1:A:469:VAL:HG22	2.01	0.42
1:B:251:VAL:CG1	1:B:355:GLU:HG3	2.45	0.42
1:B:431:LEU:O	1:B:432:MET:HB2	2.18	0.42
1:B:464:SER:HA	1:B:467:GLU:HG2	2.01	0.42
1:D:157:LYS:HE2	1:D:157:LYS:N	2.34	0.42
1:E:7:HIS:HB2	1:E:110:HIS:CE1	2.54	0.42
1:E:137:THR:OG1	1:E:208:PHE:CD2	2.72	0.42
1:E:371:TRP:HA	1:E:374:THR:OG1	2.19	0.42
1:F:124:ILE:O	1:F:127:ILE:N	2.52	0.42
1:F:151:TYR:HD2	1:F:155:PHE:CE2	2.37	0.42
1:G:399:MET:O	1:G:404:LEU:HD13	2.19	0.42
1:A:54:LEU:HD12	1:A:68:ILE:CD1	2.23	0.42
1:A:139:HIS:CE1	1:A:141:THR:O	2.72	0.42
1:A:406:VAL:O	1:A:406:VAL:HG22	2.19	0.42
1:C:101:ILE:O	1:C:105:ILE:HG13	2.20	0.42
1:E:119:ILE:CD1	1:E:120:PHE:CE1	2.96	0.42
1:E:431:LEU:C	1:E:431:LEU:CD2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:290:LEU:HD23	1:F:290:LEU:O	2.18	0.42
1:G:91:ARG:NE	1:G:197:GLU:HG3	2.33	0.42
1:B:409:ARG:HB2	1:B:410:PRO:HD2	2.01	0.42
2:B:501:U2F:O4'	2:B:501:U2F:C5'	2.56	0.42
1:C:332:LEU:CD1	1:C:333:PRO:O	2.66	0.42
1:C:350:TRP:CZ2	2:C:501:U2F:C8'	3.02	0.42
1:E:166:LEU:HD13	1:E:167:LYS:N	2.33	0.42
1:E:192:ASP:O	1:E:194:GLN:N	2.42	0.42
1:F:125:LEU:HB3	1:F:126:PRO:HD3	2.01	0.42
1:F:143:ALA:HA	1:F:213:ILE:CD1	2.49	0.42
1:A:115:LEU:CD2	1:A:128:ALA:CB	2.69	0.42
1:A:290:LEU:HA	1:A:424:ILE:HD13	2.02	0.42
1:B:371:TRP:O	1:B:375:VAL:HG13	2.20	0.42
1:B:442:GLU:O	1:B:446:LYS:HD2	2.19	0.42
1:C:273:PHE:HE2	1:C:353:GLN:HB2	1.85	0.42
1:D:301:PHE:CZ	1:D:344:GLY:HA3	2.53	0.42
1:E:21:PRO:HA	1:E:24:VAL:HG22	2.01	0.42
1:E:244:ILE:HG23	1:E:465:ILE:HD11	2.00	0.42
1:E:249:ARG:CZ	1:E:354:VAL:CG2	2.97	0.42
1:E:409:ARG:HB2	1:E:410:PRO:HD2	2.00	0.42
1:A:209:ASP:CG	1:A:475:ARG:HH12	2.27	0.42
1:B:142:THR:CG2	1:B:399:MET:HE1	2.44	0.42
1:C:76:ILE:HD11	1:C:93:LEU:CD2	2.49	0.42
1:D:98:LEU:N	1:D:99:PRO:HD2	2.34	0.42
1:E:213:ILE:CG2	1:E:215:THR:HG22	2.47	0.42
1:F:7:HIS:HD2	1:F:112:PRO:HA	1.83	0.42
1:F:124:ILE:O	1:F:125:LEU:C	2.62	0.42
1:G:108:MET:HE2	1:G:112:PRO:HD3	2.01	0.42
1:G:137:THR:HG23	1:G:208:PHE:CG	2.54	0.42
1:B:95:ARG:CA	1:B:98:LEU:HD23	2.49	0.42
1:B:171:LYS:O	1:B:171:LYS:HG3	2.19	0.42
1:C:376:GLU:OE2	2:C:501:U2F:O6'	2.37	0.42
1:D:119:ILE:HG23	1:D:120:PHE:CD2	2.55	0.42
1:D:201:LEU:C	1:D:201:LEU:CD1	2.92	0.42
1:D:290:LEU:CD2	1:D:294:LEU:CD1	2.97	0.42
1:F:95:ARG:CA	1:F:98:LEU:HD23	2.48	0.42
1:G:401:THR:HG22	1:G:407:ALA:O	2.19	0.42
1:B:263:LEU:HB3	1:B:359:HIS:CD2	2.55	0.42
1:B:336:PHE:O	1:B:339:ARG:HG2	2.20	0.42
1:C:426:GLY:HA2	1:D:253:THR:HG21	2.02	0.42
1:E:14:PRO:CG	1:E:93:LEU:HD23	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:CYS:HB3	1:G:124:ILE:CD1	2.49	0.42
1:B:99:PRO:O	1:B:102:HIS:HB3	2.20	0.42
1:C:41:ALA:O	1:C:71:VAL:HG12	2.19	0.42
1:C:145:THR:HG21	1:C:392:GLU:HG3	2.02	0.42
1:D:248:ARG:HD3	1:D:379:THR:HG21	2.02	0.42
1:E:235:LEU:HD13	1:E:235:LEU:O	2.19	0.42
1:E:250:LYS:HD3	1:E:250:LYS:HA	1.92	0.42
1:E:304:VAL:HG13	1:E:349:MET:O	2.19	0.42
1:E:328:MET:HE2	1:E:348:PRO:HA	2.02	0.42
1:F:212:LEU:N	1:F:212:LEU:HD12	2.35	0.42
1:B:387:TRP:CH2	1:B:419:VAL:HG21	2.54	0.42
1:C:98:LEU:N	1:C:99:PRO:HD2	2.35	0.42
1:C:301:PHE:CZ	1:C:344:GLY:HA3	2.53	0.42
1:D:48:SER:O	1:D:49:ALA:C	2.63	0.42
1:F:20:ILE:HG21	1:F:249:ARG:CD	2.49	0.42
1:A:98:LEU:N	1:A:99:PRO:HD2	2.35	0.42
1:A:371:TRP:HA	1:A:374:THR:OG1	2.19	0.42
1:C:290:LEU:HA	1:C:424:ILE:HD13	2.02	0.42
1:D:371:TRP:HA	1:D:374:THR:OG1	2.19	0.42
1:F:129:GLU:O	1:F:132:ASN:N	2.48	0.42
1:F:145:THR:HG21	1:F:392:GLU:HG3	2.00	0.42
1:G:359:HIS:ND1	1:G:361:SER:OG	2.45	0.42
1:C:401:THR:HG21	1:C:409:ARG:HD3	2.02	0.41
1:E:7:HIS:ND1	1:E:112:PRO:HA	2.35	0.41
1:F:231:GLU:HG2	1:F:232:LYS:N	2.34	0.41
1:G:145:THR:HG21	1:G:392:GLU:HG3	2.02	0.41
1:G:167:LYS:HE3	1:G:167:LYS:HB3	1.55	0.41
1:A:13:SER:CB	1:A:14:PRO:CD	2.99	0.41
1:B:432:MET:HB3	1:B:432:MET:HE3	1.38	0.41
1:C:396:ASN:O	1:C:400:LEU:HG	2.20	0.41
1:D:330:GLU:HG3	1:D:331:TYR:CD2	2.55	0.41
1:E:19:LEU:C	1:E:22:VAL:HG22	2.43	0.41
1:G:90:LEU:CD1	1:G:120:PHE:CE1	3.02	0.41
1:G:285:LYS:CE	1:G:285:LYS:CA	2.95	0.41
1:G:352:ASN:HD22	1:G:352:ASN:N	2.18	0.41
1:B:201:LEU:C	1:B:201:LEU:CD1	2.92	0.41
1:B:209:ASP:C	1:B:239:VAL:CG1	2.93	0.41
1:D:104:THR:O	1:D:108:MET:HG3	2.19	0.41
1:D:325:THR:HA	1:D:349:MET:HE3	2.01	0.41
1:E:98:LEU:N	1:E:99:PRO:HD2	2.34	0.41
1:E:119:ILE:HG13	1:E:120:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:LEU:HD13	1:E:416:LYS:CD	2.50	0.41
1:G:137:THR:HG23	1:G:208:PHE:CE2	2.54	0.41
1:G:141:THR:HG23	1:G:142:THR:H	1.84	0.41
1:G:426:GLY:O	1:G:427:MET:C	2.62	0.41
1:G:473:ARG:C	1:G:475:ARG:H	2.27	0.41
1:A:94:VAL:O	1:A:97:ALA:N	2.53	0.41
1:A:145:THR:HG21	1:A:392:GLU:HG3	2.02	0.41
1:A:429:ARG:CZ	1:A:433:GLN:NE2	2.77	0.41
1:C:115:LEU:HD13	1:C:133:ILE:HG21	2.01	0.41
1:D:106:ALA:O	1:D:107:SER:CB	2.67	0.41
1:F:401:THR:HG21	1:F:409:ARG:HD3	2.02	0.41
1:G:20:ILE:HG21	1:G:249:ARG:HD3	2.02	0.41
1:G:88:THR:O	1:G:89:GLN:C	2.63	0.41
1:A:51:THR:O	1:A:54:LEU:HB3	2.20	0.41
1:A:423:GLU:O	1:A:427:MET:HG3	2.21	0.41
1:D:146:LEU:CD2	1:D:213:ILE:HD11	2.50	0.41
1:F:281:THR:CG2	1:F:309:SER:HB3	2.50	0.41
1:G:341:LYS:O	1:G:342:ASP:HB2	2.21	0.41
1:B:201:LEU:HD13	1:B:201:LEU:O	2.20	0.41
1:C:52:GLU:H	1:C:52:GLU:HG3	1.50	0.41
1:C:435:LYS:NZ	1:D:357:LEU:O	2.53	0.41
1:F:79:LEU:HB3	1:F:92:LEU:HD13	2.02	0.41
1:G:146:LEU:C	1:G:146:LEU:HD13	2.45	0.41
1:B:159:ILE:N	1:B:159:ILE:HD12	2.36	0.41
1:B:253:THR:O	1:B:254:THR:C	2.64	0.41
1:D:213:ILE:HG21	1:D:213:ILE:HD13	1.84	0.41
1:F:290:LEU:HA	1:F:424:ILE:HD13	2.03	0.41
1:G:105:ILE:O	1:G:106:ALA:HB3	2.21	0.41
1:A:54:LEU:HA	1:A:57:THR:HG22	2.02	0.41
1:A:249:ARG:CZ	1:A:354:VAL:CG2	2.99	0.41
1:B:255:LEU:HD13	1:B:260:ILE:HG13	2.03	0.41
1:C:61:ASN:OD1	1:C:61:ASN:C	2.64	0.41
1:C:138:TYR:O	1:C:140:PRO:HD3	2.21	0.41
1:C:159:ILE:HD13	1:C:160:GLU:H	1.85	0.41
1:D:119:ILE:HG13	1:D:205:TYR:OH	2.21	0.41
1:A:35:ILE:HD11	1:A:469:VAL:HG12	2.02	0.41
1:B:178:LEU:HD22	1:B:395:MET:HE3	2.03	0.41
1:B:336:PHE:CA	1:B:339:ARG:NH1	2.83	0.41
1:C:117:VAL:HG12	1:C:118:ASP:O	2.21	0.41
1:C:371:TRP:HA	1:C:374:THR:OG1	2.21	0.41
1:D:105:ILE:O	1:D:108:MET:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:LEU:HA	1:D:424:ILE:HD13	2.02	0.41
1:E:154:VAL:O	1:E:158:GLU:HG2	2.20	0.41
1:E:178:LEU:HD22	1:E:395:MET:HE3	2.03	0.41
1:E:237:LEU:HD12	1:E:239:VAL:O	2.21	0.41
1:F:26:GLY:O	1:F:37:ILE:HD12	2.21	0.41
1:G:69:ILE:O	1:G:69:ILE:HG22	2.20	0.41
1:G:371:TRP:HA	1:G:374:THR:OG1	2.20	0.41
1:G:396:ASN:O	1:G:400:LEU:HG	2.21	0.41
1:A:106:ALA:O	1:A:107:SER:CB	2.69	0.41
1:B:255:LEU:HA	1:B:255:LEU:HD23	1.84	0.41
1:B:471:ASP:O	1:B:475:ARG:HG2	2.21	0.41
1:C:455:LEU:HD23	1:C:455:LEU:HA	1.83	0.41
1:D:471:ASP:O	1:D:475:ARG:HG2	2.21	0.41
1:E:76:ILE:HG23	1:E:79:LEU:HB2	2.02	0.41
1:G:98:LEU:N	1:G:99:PRO:HD2	2.36	0.41
1:G:231:GLU:O	1:G:235:LEU:HG	2.21	0.41
1:G:235:LEU:HA	1:G:238:LYS:HZ2	1.84	0.41
1:A:118:ASP:O	1:A:119:ILE:C	2.64	0.40
1:B:255:LEU:CD1	1:B:260:ILE:HG13	2.51	0.40
1:C:341:LYS:O	1:C:342:ASP:HB2	2.21	0.40
1:E:438:LYS:HD2	1:E:438:LYS:H	1.84	0.40
1:G:179:ARG:CD	1:G:180:PRO:HD2	2.50	0.40
1:A:105:ILE:HA	1:A:108:MET:CG	2.51	0.40
1:B:326:ARG:HB3	1:B:331:TYR:CE1	2.56	0.40
1:C:180:PRO:O	1:C:183:VAL:HG13	2.21	0.40
1:E:146:LEU:C	1:E:146:LEU:CD1	2.93	0.40
1:E:189:ASP:C	1:E:191:SER:N	2.79	0.40
1:E:201:LEU:C	1:E:201:LEU:CD1	2.92	0.40
1:F:306:ARG:HB3	1:F:307:PRO:HD2	2.03	0.40
1:F:396:ASN:O	1:F:400:LEU:HG	2.21	0.40
1:G:266:GLN:HG3	1:G:300:LYS:HD3	2.03	0.40
1:C:385:ILE:HG13	1:C:431:LEU:HD22	2.03	0.40
1:E:101:ILE:O	1:E:104:THR:OG1	2.39	0.40
1:E:263:LEU:CB	1:E:359:HIS:ND1	2.85	0.40
1:G:76:ILE:HG23	1:G:80:ILE:HD12	2.04	0.40
1:G:94:VAL:C	1:G:96:GLU:N	2.77	0.40
1:G:366:LEU:HD11	1:G:387:TRP:HE3	1.86	0.40
1:B:138:TYR:O	1:B:140:PRO:HD3	2.22	0.40
1:C:71:VAL:HG21	1:C:101:ILE:HD13	2.04	0.40
1:E:94:VAL:HG23	1:E:95:ARG:N	2.37	0.40
1:E:189:ASP:C	1:E:191:SER:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:193:GLN:O	1:E:194:GLN:C	2.64	0.40
1:E:255:LEU:H	1:E:255:LEU:HG	1.56	0.40
1:F:253:THR:CG2	1:G:425:GLN:NE2	2.84	0.40
1:F:328:MET:HA	1:F:331:TYR:CZ	2.57	0.40
1:G:90:LEU:HD13	1:G:120:PHE:CE1	2.57	0.40
1:A:54:LEU:O	1:A:57:THR:HG22	2.21	0.40
1:B:180:PRO:O	1:B:183:VAL:HG13	2.22	0.40
1:B:385:ILE:CG2	1:B:427:MET:HE2	2.52	0.40
1:C:212:LEU:CD2	1:C:244:ILE:HD12	2.51	0.40
1:E:166:LEU:HD22	1:E:166:LEU:HA	1.92	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:GLN:NE2	1:B:264:ASP:OD2[2_646]	2.07	0.13

5.3 Torsion angles

5.3.1 Protein backbone

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	449/479 (94%)	418 (93%)	30 (7%)	1 (0%)	43	71
1	B	455/479 (95%)	424 (93%)	31 (7%)	0	100	100
1	C	456/479 (95%)	420 (92%)	36 (8%)	0	100	100
1	D	456/479 (95%)	422 (92%)	33 (7%)	1 (0%)	43	71
1	E	455/479 (95%)	423 (93%)	32 (7%)	0	100	100
1	F	455/479 (95%)	422 (93%)	33 (7%)	0	100	100
1	G	456/479 (95%)	405 (89%)	50 (11%)	1 (0%)	43	71
All	All	3182/3353 (95%)	2934 (92%)	245 (8%)	3 (0%)	48	77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	SER
1	D	73	SER
1	G	77	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	408/425 (96%)	374 (92%)	34 (8%)	10	34
1	B	412/425 (97%)	386 (94%)	26 (6%)	16	43
1	C	413/425 (97%)	382 (92%)	31 (8%)	12	38
1	D	413/425 (97%)	379 (92%)	34 (8%)	10	34
1	E	412/425 (97%)	381 (92%)	31 (8%)	12	38
1	F	412/425 (97%)	365 (89%)	47 (11%)	5	22
1	G	413/425 (97%)	359 (87%)	54 (13%)	4	17
All	All	2883/2975 (97%)	2626 (91%)	257 (9%)	9	31

All (257) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	38	THR
1	A	44	THR
1	A	45	THR
1	A	47	SER
1	A	54	LEU
1	A	59	LEU
1	A	66	ILE
1	A	80	ILE
1	A	93	LEU
1	A	118	ASP
1	A	119	ILE
1	A	123	GLN

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Mol	Chain	Res	Type
1	A	127	ILE
1	A	175	CYS
1	A	199	VAL
1	A	211	ILE
1	A	233	LEU
1	A	235	LEU
1	A	258	GLU
1	A	305	VAL
1	A	326	ARG
1	A	327	ASP
1	A	328	MET
1	A	330	GLU
1	A	331	TYR
1	A	334	GLU
1	A	354	VAL
1	A	358	SER
1	A	395	MET
1	A	432	MET
1	A	450	SER
1	A	461	SER
1	A	465	ILE
1	B	24	VAL
1	B	59	LEU
1	B	60	THR
1	B	64	LYS
1	B	65	THR
1	B	66	ILE
1	B	104	THR
1	B	117	VAL
1	B	135	LYS
1	B	142	THR
1	B	167	LYS
1	B	175	CYS
1	B	192	ASP
1	B	194	GLN
1	B	237	LEU
1	B	330	GLU
1	B	331	TYR
1	B	419	VAL
1	B	428	VAL
1	B	430	ILE
1	B	432	MET

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Mol	Chain	Res	Type
1	B	433	GLN
1	B	439	ARG
1	B	441	LYS
1	B	460	SER
1	B	472	ILE
1	C	47	SER
1	C	52	GLU
1	C	59	LEU
1	C	69	ILE
1	C	82	SER
1	C	86	ILE
1	C	101	ILE
1	C	117	VAL
1	C	124	ILE
1	C	159	ILE
1	C	160	GLU
1	C	170	LEU
1	C	172	ILE
1	C	175	CYS
1	C	176	LYS
1	C	237	LEU
1	C	238	LYS
1	C	239	VAL
1	C	241	VAL
1	C	248	ARG
1	C	305	VAL
1	C	331	TYR
1	C	337	LEU
1	C	349	MET
1	C	354	VAL
1	C	361	SER
1	C	415	THR
1	C	420	LYS
1	C	428	VAL
1	C	450	SER
1	C	472	ILE
1	D	37	ILE
1	D	38	THR
1	D	39	ILE
1	D	54	LEU
1	D	59	LEU
1	D	74	VAL

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Mol	Chain	Res	Type
1	D	82	SER
1	D	93	LEU
1	D	100	LYS
1	D	103	SER
1	D	109	THR
1	D	117	VAL
1	D	142	THR
1	D	157	LYS
1	D	164	VAL
1	D	165	GLU
1	D	166	LEU
1	D	167	LYS
1	D	168	GLU
1	D	193	GLN
1	D	231	GLU
1	D	237	LEU
1	D	284	THR
1	D	326	ARG
1	D	327	ASP
1	D	333	PRO
1	D	341	LYS
1	D	354	VAL
1	D	361	SER
1	D	387	TRP
1	D	396	ASN
1	D	418	LEU
1	D	450	SER
1	D	468	LEU
1	E	37	ILE
1	E	39	ILE
1	E	80	ILE
1	E	105	ILE
1	E	111	ARG
1	E	115	LEU
1	E	116	ILE
1	E	119	ILE
1	E	166	LEU
1	E	168	GLU
1	E	170	LEU
1	E	175	CYS
1	E	211	ILE
1	E	213	ILE

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Mol	Chain	Res	Type
1	E	237	LEU
1	E	255	LEU
1	E	296	LEU
1	E	326	ARG
1	E	328	MET
1	E	329	SER
1	E	343	MET
1	E	349	MET
1	E	354	VAL
1	E	361	SER
1	E	404	LEU
1	E	438	LYS
1	E	450	SER
1	E	468	LEU
1	E	470	LYS
1	E	476	GLU
1	E	477	LEU
1	F	38	THR
1	F	39	ILE
1	F	60	THR
1	F	62	GLU
1	F	74	VAL
1	F	75	ASP
1	F	76	ILE
1	F	77	SER
1	F	79	LEU
1	F	100	LYS
1	F	107	SER
1	F	113	ASP
1	F	117	VAL
1	F	124	ILE
1	F	125	LEU
1	F	127	ILE
1	F	133	ILE
1	F	160	GLU
1	F	166	LEU
1	F	172	ILE
1	F	175	CYS
1	F	194	GLN
1	F	201	LEU
1	F	219	LEU
1	F	222	GLU

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Mol	Chain	Res	Type
1	F	224	ILE
1	F	237	LEU
1	F	255	LEU
1	F	290	LEU
1	F	328	MET
1	F	329	SER
1	F	331	TYR
1	F	341	LYS
1	F	349	MET
1	F	354	VAL
1	F	361	SER
1	F	399	MET
1	F	419	VAL
1	F	428	VAL
1	F	447	LEU
1	F	461	SER
1	F	468	LEU
1	F	470	LYS
1	F	472	ILE
1	F	473	ARG
1	F	475	ARG
1	F	477	LEU
1	G	5	GLN
1	G	6	LEU
1	G	8	VAL
1	G	10	ILE
1	G	19	LEU
1	G	35	ILE
1	G	42	ILE
1	G	43	THR
1	G	50	GLU
1	G	54	LEU
1	G	55	LYS
1	G	62	GLU
1	G	63	GLU
1	G	64	LYS
1	G	65	THR
1	G	74	VAL
1	G	77	SER
1	G	84	THR
1	G	86	ILE
1	G	91	ARG

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Mol	Chain	Res	Type
1	G	94	VAL
1	G	98	LEU
1	G	105	ILE
1	G	113	ASP
1	G	119	ILE
1	G	127	ILE
1	G	141	THR
1	G	142	THR
1	G	146	LEU
1	G	166	LEU
1	G	167	LYS
1	G	175	CYS
1	G	199	VAL
1	G	213	ILE
1	G	237	LEU
1	G	251	VAL
1	G	285	LYS
1	G	296	LEU
1	G	327	ASP
1	G	328	MET
1	G	329	SER
1	G	330	GLU
1	G	345	LEU
1	G	347	VAL
1	G	352	ASN
1	G	361	SER
1	G	401	THR
1	G	428	VAL
1	G	450	SER
1	G	460	SER
1	G	469	VAL
1	G	473	ARG
1	G	475	ARG
1	G	477	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	HIS
1	A	256	ASN
1	A	299	GLN
1	A	368	HIS

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Mol	Chain	Res	Type
1	A	372	ASN
1	B	5	GLN
1	B	18	HIS
1	B	110	HIS
1	B	193	GLN
1	B	194	GLN
1	B	353	GLN
1	B	463	ASN
1	C	5	GLN
1	C	18	HIS
1	C	27	ASN
1	C	34	ASN
1	C	78	HIS
1	C	102	HIS
1	C	123	GLN
1	C	268	ASN
1	C	286	GLN
1	C	299	GLN
1	C	352	ASN
1	C	372	ASN
1	C	453	ASN
1	D	18	HIS
1	D	27	ASN
1	D	34	ASN
1	D	61	ASN
1	D	78	HIS
1	D	123	GLN
1	D	286	GLN
1	D	299	GLN
1	D	368	HIS
1	D	396	ASN
1	D	463	ASN
1	E	5	GLN
1	E	27	ASN
1	E	32	HIS
1	E	102	HIS
1	E	110	HIS
1	E	261	GLN
1	E	286	GLN
1	E	299	GLN
1	E	368	HIS
1	E	372	ASN

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Mol	Chain	Res	Type
1	F	5	GLN
1	F	18	HIS
1	F	27	ASN
1	F	33	HIS
1	F	61	ASN
1	F	89	GLN
1	F	110	HIS
1	F	153	GLN
1	F	268	ASN
1	F	286	GLN
1	F	372	ASN
1	F	425	GLN
1	F	433	GLN
1	F	453	ASN
1	G	27	ASN
1	G	32	HIS
1	G	61	ASN
1	G	110	HIS
1	G	225	ASN
1	G	286	GLN
1	G	298	GLN
1	G	299	GLN
1	G	352	ASN
1	G	368	HIS
1	G	372	ASN
1	G	425	GLN
1	G	433	GLN
1	G	463	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	E	501	-	37,38,38	3.37	21 (56%)	53,58,58	2.09	18 (33%)
3	T83	C	502	-	15,15,15	0.51	0	21,21,21	0.95	2 (9%)
2	U2F	C	501	-	37,38,38	3.71	20 (54%)	53,58,58	1.91	8 (15%)
3	T83	B	502	-	15,15,15	0.49	0	21,21,21	0.94	2 (9%)
2	U2F	A	501	-	37,38,38	0.52	0	53,58,58	0.57	0
2	U2F	F	501	-	37,38,38	3.64	20 (54%)	53,58,58	1.88	12 (22%)
3	T83	F	502	-	15,15,15	0.50	0	21,21,21	0.93	2 (9%)
2	U2F	G	501	-	37,38,38	3.54	22 (59%)	53,58,58	1.84	11 (20%)
3	T83	D	502	-	15,15,15	0.54	0	21,21,21	0.92	2 (9%)
3	T83	A	502	-	15,15,15	0.62	0	21,21,21	1.02	2 (9%)
2	U2F	B	501	-	37,38,38	3.41	22 (59%)	53,58,58	1.69	13 (24%)
2	U2F	D	501	-	37,38,38	3.42	20 (54%)	53,58,58	1.82	13 (24%)

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	E	501	-	-	14/22/59/59	0/3/3/3
3	T83	C	502	-	-	2/2/2/2	0/2/2/2
2	U2F	C	501	-	-	7/22/59/59	0/3/3/3
3	T83	B	502	-	-	2/2/2/2	0/2/2/2
2	U2F	A	501	-	-	7/22/59/59	0/3/3/3
2	U2F	F	501	-	-	7/22/59/59	0/3/3/3
3	T83	F	502	-	-	2/2/2/2	0/2/2/2
2	U2F	G	501	-	-	7/22/59/59	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	T83	D	502	-	-	2/2/2/2	0/2/2/2
3	T83	A	502	-	-	2/2/2/2	0/2/2/2
2	U2F	B	501	-	-	7/22/59/59	0/3/3/3
2	U2F	D	501	-	-	8/22/59/59	0/3/3/3

All (125) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	501	U2F	O4'-C4'	9.88	1.67	1.45
2	F	501	U2F	O4'-C4'	9.85	1.66	1.45
2	D	501	U2F	O4'-C4'	9.70	1.66	1.45
2	B	501	U2F	O4'-C4'	9.47	1.66	1.45
2	E	501	U2F	O4'-C4'	9.38	1.65	1.45
2	C	501	U2F	O4'-C4'	9.33	1.65	1.45
2	C	501	U2F	C2-C3	-8.54	1.44	1.52
2	B	501	U2F	O7'-C7'	7.91	1.39	1.24
2	G	501	U2F	O7'-C7'	7.73	1.39	1.24
2	F	501	U2F	O7'-C7'	7.71	1.39	1.24
2	D	501	U2F	O7'-C7'	7.38	1.38	1.24
2	F	501	U2F	C2-C3	-7.14	1.45	1.52
2	C	501	U2F	O7'-C7'	6.98	1.38	1.24
2	C	501	U2F	C3'-C4'	-6.95	1.35	1.53
2	D	501	U2F	C3'-C4'	-6.78	1.35	1.53
2	E	501	U2F	C3'-C4'	-6.70	1.36	1.53
2	F	501	U2F	C3'-C4'	-6.69	1.36	1.53
2	B	501	U2F	C3'-C4'	-6.67	1.36	1.53
2	D	501	U2F	C2-C3	-6.67	1.46	1.52
2	E	501	U2F	C2-C3	-6.66	1.46	1.52
2	E	501	U2F	O7'-C7'	6.64	1.37	1.24
2	G	501	U2F	C2-C3	-6.55	1.46	1.52
2	B	501	U2F	C2-C3	-6.42	1.46	1.52
2	G	501	U2F	C3'-C4'	-6.32	1.37	1.53
2	C	501	U2F	PA-O3A	5.93	1.65	1.59
2	G	501	U2F	PA-O3A	5.58	1.65	1.59
2	G	501	U2F	O4'-C1'	-5.37	1.29	1.42
2	F	501	U2F	O4'-C1'	-5.33	1.29	1.42
2	F	501	U2F	PA-O3A	5.30	1.65	1.59
2	C	501	U2F	PB-O3A	5.24	1.65	1.59
2	E	501	U2F	O4'-C1'	-5.02	1.30	1.42
2	C	501	U2F	O4'-C1'	-4.98	1.30	1.42
2	D	501	U2F	O4'-C1'	-4.91	1.30	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	501	U2F	PB-O3A	4.89	1.64	1.59
2	B	501	U2F	O4'-C1'	-4.81	1.30	1.42
2	C	501	U2F	C7'-N3	-4.75	1.30	1.38
2	E	501	U2F	PA-O3A	4.53	1.64	1.59
2	F	501	U2F	O5-C5	4.51	1.55	1.44
2	D	501	U2F	O5-C5	4.50	1.55	1.44
2	C	501	U2F	O2'-C2'	-4.47	1.31	1.43
2	F	501	U2F	O2'-C2'	-4.40	1.32	1.43
2	B	501	U2F	O2'-C2'	-4.27	1.32	1.43
2	G	501	U2F	PB-O3A	4.23	1.64	1.59
2	E	501	U2F	O2'-C2'	-4.10	1.32	1.43
2	E	501	U2F	O5-C5	4.06	1.54	1.44
2	B	501	U2F	PA-O3A	4.05	1.63	1.59
2	F	501	U2F	C7'-N3	-4.04	1.31	1.38
2	C	501	U2F	O5-C5	3.99	1.54	1.44
2	D	501	U2F	O2'-C2'	-3.99	1.33	1.43
2	G	501	U2F	O2'-C2'	-3.92	1.33	1.43
2	D	501	U2F	C7'-N3	-3.92	1.31	1.38
2	B	501	U2F	O5-C5	3.89	1.53	1.44
2	G	501	U2F	C6'-N1	-3.81	1.32	1.38
2	G	501	U2F	O5-C5	3.80	1.53	1.44
2	B	501	U2F	PB-O3A	3.72	1.63	1.59
2	F	501	U2F	C6'-N1	-3.67	1.32	1.38
2	G	501	U2F	C7'-N3	-3.63	1.32	1.38
2	B	501	U2F	C6'-N1	-3.53	1.32	1.38
2	D	501	U2F	C6'-N1	-3.52	1.32	1.38
2	C	501	U2F	C6'-N3	-3.45	1.32	1.38
2	B	501	U2F	C7'-N3	-3.45	1.32	1.38
2	D	501	U2F	PB-O3A	3.43	1.63	1.59
2	F	501	U2F	PB-O1	3.42	1.69	1.59
2	E	501	U2F	C7'-N3	-3.40	1.32	1.38
2	E	501	U2F	C2-C1	-3.40	1.49	1.52
2	C	501	U2F	C2'-C1'	3.37	1.64	1.53
2	D	501	U2F	PB-O1	3.29	1.69	1.59
2	E	501	U2F	C6'-N1	-3.25	1.33	1.38
2	D	501	U2F	PA-O3A	3.25	1.63	1.59
2	G	501	U2F	PB-O1	3.19	1.68	1.59
2	C	501	U2F	C6'-N1	-3.17	1.33	1.38
2	B	501	U2F	PB-O1	3.06	1.68	1.59
2	F	501	U2F	O5-C1	3.04	1.49	1.41
2	E	501	U2F	F1-C2	3.02	1.46	1.40
2	C	501	U2F	O5-C1	3.00	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	U2F	PB-O1	3.00	1.68	1.59
2	E	501	U2F	PB-O3A	2.88	1.62	1.59
2	B	501	U2F	F1-C2	2.88	1.46	1.40
2	C	501	U2F	F1-C2	2.87	1.46	1.40
2	E	501	U2F	C6'-N3	-2.83	1.33	1.38
2	E	501	U2F	PB-O1	2.81	1.67	1.59
2	G	501	U2F	F1-C2	2.81	1.45	1.40
2	G	501	U2F	C2'-C1'	2.78	1.62	1.53
2	F	501	U2F	O3'-C3'	2.76	1.49	1.43
2	D	501	U2F	O5-C1	2.75	1.48	1.41
2	E	501	U2F	O5-C1	2.74	1.48	1.41
2	D	501	U2F	F1-C2	2.72	1.45	1.40
2	D	501	U2F	C2'-C1'	2.65	1.61	1.53
2	C	501	U2F	C2-C1	-2.65	1.49	1.52
2	C	501	U2F	O6'-C6'	-2.64	1.18	1.23
2	E	501	U2F	C2'-C1'	2.61	1.61	1.53
2	G	501	U2F	C2-C1	-2.60	1.49	1.52
2	F	501	U2F	F1-C2	2.59	1.45	1.40
2	F	501	U2F	O6'-C6'	-2.53	1.18	1.23
2	G	501	U2F	O3'-C3'	2.51	1.49	1.43
2	D	501	U2F	C6'-N3	-2.50	1.33	1.38
2	B	501	U2F	C2'-C1'	2.47	1.61	1.53
2	C	501	U2F	O3'-C3'	2.45	1.49	1.43
2	D	501	U2F	O3'-C3'	2.44	1.49	1.43
2	B	501	U2F	O3'-C3'	2.43	1.49	1.43
2	G	501	U2F	O5-C1	2.42	1.48	1.41
2	E	501	U2F	O3-C3	2.39	1.48	1.43
2	B	501	U2F	O5-C1	2.38	1.48	1.41
2	F	501	U2F	C2'-C1'	2.37	1.60	1.53
2	E	501	U2F	C8'-C7'	-2.36	1.38	1.43
2	F	501	U2F	C6'-N3	-2.35	1.33	1.38
2	G	501	U2F	O6'-C6'	-2.34	1.18	1.23
2	G	501	U2F	O3-C3	2.33	1.48	1.43
2	B	501	U2F	C6-C5	-2.29	1.44	1.51
2	B	501	U2F	O3-C3	2.29	1.48	1.43
2	G	501	U2F	PA-O5'	2.27	1.68	1.59
2	E	501	U2F	O3'-C3'	2.25	1.48	1.43
2	D	501	U2F	C8'-C7'	-2.22	1.38	1.43
2	B	501	U2F	C2-C1	-2.21	1.50	1.52
2	G	501	U2F	C9'-C8'	2.17	1.40	1.35
2	B	501	U2F	C6'-N3	-2.17	1.34	1.38
2	D	501	U2F	PA-O5'	2.16	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	U2F	PA-O5'	2.11	1.67	1.59
2	B	501	U2F	C8'-C7'	-2.11	1.39	1.43
2	F	501	U2F	C2-C1	-2.09	1.50	1.52
2	F	501	U2F	C9'-N1	-2.07	1.33	1.38
2	D	501	U2F	C2-C1	-2.06	1.50	1.52
2	C	501	U2F	C6-C5	-2.05	1.44	1.51
2	G	501	U2F	C6-C5	-2.05	1.44	1.51
2	B	501	U2F	O6'-C6'	-2.04	1.19	1.23

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	U2F	N3-C6'-N1	7.24	124.32	114.89
2	F	501	U2F	N3-C6'-N1	7.17	124.22	114.89
2	G	501	U2F	N3-C6'-N1	6.98	123.98	114.89
2	C	501	U2F	C7'-N3-C6'	-6.44	118.62	126.61
2	B	501	U2F	N3-C6'-N1	6.24	123.01	114.89
2	F	501	U2F	C7'-N3-C6'	-5.96	119.21	126.61
2	D	501	U2F	N3-C6'-N1	5.69	122.29	114.89
2	G	501	U2F	C7'-N3-C6'	-5.12	120.26	126.61
2	E	501	U2F	C8'-C7'-N3	5.01	121.82	114.80
2	D	501	U2F	C1-O5-C5	4.76	123.02	113.72
2	E	501	U2F	C2'-C3'-C4'	-4.65	93.62	102.61
2	E	501	U2F	C7'-N3-C6'	-4.63	120.87	126.61
2	B	501	U2F	C7'-N3-C6'	-4.46	121.07	126.61
2	D	501	U2F	C7'-N3-C6'	-4.45	121.09	126.61
2	E	501	U2F	O7'-C7'-C8'	-4.32	117.72	125.16
2	C	501	U2F	C8'-C7'-N3	4.16	120.63	114.80
2	F	501	U2F	C1-O5-C5	4.13	121.79	113.72
2	E	501	U2F	N3-C6'-N1	3.89	119.95	114.89
2	E	501	U2F	O5-C5-C4	-3.83	102.81	109.70
2	D	501	U2F	C1-C2-C3	3.78	116.07	110.54
2	C	501	U2F	O6'-C6'-N3	-3.76	114.56	121.49
2	B	501	U2F	O7'-C7'-C8'	-3.56	119.02	125.16
2	E	501	U2F	C1'-N1-C6'	3.40	123.69	117.59
2	E	501	U2F	O2A-PA-O3A	3.30	116.19	107.27
2	D	501	U2F	C8'-C7'-N3	3.17	119.24	114.80
2	E	501	U2F	O3'-C3'-C4'	3.14	120.09	111.08
2	E	501	U2F	C3-C4-C5	3.08	115.83	110.23
3	A	502	T83	OAC-CAJ-CAK	3.07	127.35	120.13
2	E	501	U2F	O3A-PA-O1A	-3.06	101.48	110.70
2	C	501	U2F	C1-O5-C5	3.06	119.69	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	U2F	O6'-C6'-N1	-3.06	118.82	122.80
2	D	501	U2F	O7'-C7'-C8'	-3.05	119.90	125.16
2	F	501	U2F	O6'-C6'-N3	-3.01	115.93	121.49
2	G	501	U2F	C3-C4-C5	3.00	115.67	110.23
2	E	501	U2F	C9'-C8'-C7'	-2.93	115.78	119.53
2	F	501	U2F	F1-C2-C1	2.93	110.99	107.62
2	E	501	U2F	C4'-O4'-C1'	-2.85	103.18	109.47
2	G	501	U2F	O7'-C7'-C8'	-2.83	120.28	125.16
3	C	502	T83	OAC-CAJ-CAK	2.82	126.75	120.13
3	B	502	T83	OAC-CAJ-CAK	2.78	126.67	120.13
2	F	501	U2F	C8'-C7'-N3	2.76	118.67	114.80
2	D	501	U2F	F1-C2-C1	2.76	110.80	107.62
2	G	501	U2F	O4'-C1'-C2'	-2.76	100.72	106.62
2	C	501	U2F	F1-C2-C1	2.72	110.75	107.62
3	D	502	T83	OAC-CAJ-CAK	2.71	126.49	120.13
3	F	502	T83	OAC-CAJ-CAK	2.69	126.44	120.13
2	D	501	U2F	O6'-C6'-N3	-2.68	116.55	121.49
2	B	501	U2F	C8'-C7'-N3	2.67	118.54	114.80
3	A	502	T83	OAC-CAJ-CAF	-2.67	112.25	119.45
2	B	501	U2F	C9'-N1-C6'	-2.62	117.81	121.00
2	G	501	U2F	C8'-C7'-N3	2.61	118.45	114.80
2	F	501	U2F	C1'-N1-C6'	2.57	122.21	117.59
2	G	501	U2F	C4'-O4'-C1'	-2.52	103.89	109.47
2	D	501	U2F	C1'-N1-C6'	2.51	122.11	117.59
2	E	501	U2F	C1'-N1-C9'	-2.51	115.42	120.78
2	E	501	U2F	O6'-C6'-N3	-2.51	116.86	121.49
2	B	501	U2F	O6'-C6'-N3	-2.50	116.89	121.49
2	B	501	U2F	F1-C2-C1	2.48	110.47	107.62
3	C	502	T83	OAC-CAJ-CAF	-2.41	112.95	119.45
3	B	502	T83	OAC-CAJ-CAF	-2.38	113.04	119.45
2	G	501	U2F	C9'-N1-C6'	-2.36	118.13	121.00
2	E	501	U2F	O4-C4-C5	-2.34	103.56	109.32
3	D	502	T83	OAC-CAJ-CAF	-2.34	113.14	119.45
2	B	501	U2F	C1'-N1-C6'	2.34	121.79	117.59
3	F	502	T83	OAC-CAJ-CAF	-2.33	113.18	119.45
2	G	501	U2F	O6'-C6'-N3	-2.32	117.20	121.49
2	F	501	U2F	O1-C1-C2	2.32	112.63	108.38
2	F	501	U2F	C3'-C2'-C1'	2.27	105.76	101.46
2	F	501	U2F	O6'-C6'-N1	-2.26	119.85	122.80
2	B	501	U2F	O5-C1-O1	-2.22	108.46	111.36
2	D	501	U2F	O5-C5-C4	2.21	113.68	109.70
2	D	501	U2F	C3-C4-C5	2.19	114.20	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	U2F	O7'-C7'-N3	2.19	122.44	119.27
2	E	501	U2F	O5-C5-C6	2.18	111.85	106.44
2	C	501	U2F	C3-C4-C5	2.18	114.18	110.23
2	B	501	U2F	C3'-C2'-C1'	2.16	105.55	101.46
2	G	501	U2F	O5-C1-O1	-2.11	108.61	111.36
2	E	501	U2F	F1-C2-C1	2.09	110.03	107.62
2	C	501	U2F	O2'-C2'-C3'	-2.08	105.15	111.82
2	B	501	U2F	O6'-C6'-N1	-2.07	120.10	122.80
2	F	501	U2F	O7'-C7'-C8'	-2.06	121.61	125.16
2	D	501	U2F	O3A-PA-O1A	-2.06	104.52	110.70
2	D	501	U2F	O3-C3-C4	-2.05	105.54	110.38
2	F	501	U2F	C8'-C9'-N1	-2.04	118.53	121.84
2	B	501	U2F	O1-C1-C2	2.02	112.09	108.38

There are no chirality outliers.

All (67) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
3	F	502	T83	CAJ-CAK-OAH-CAA
3	A	502	T83	CAJ-CAK-OAH-CAA
2	A	501	U2F	C4-C5-C6-O6
2	E	501	U2F	C2'-C1'-N1-C6'
2	C	501	U2F	O4'-C4'-C5'-O5'
2	E	501	U2F	C3'-C4'-C5'-O5'
2	E	501	U2F	O5-C5-C6-O6
2	A	501	U2F	O5-C5-C6-O6
2	F	501	U2F	C4-C5-C6-O6
2	E	501	U2F	C4-C5-C6-O6
2	E	501	U2F	C2'-C1'-N1-C9'
2	C	501	U2F	C3'-C4'-C5'-O5'
2	F	501	U2F	O5-C5-C6-O6
2	E	501	U2F	O4'-C4'-C5'-O5'
2	B	501	U2F	O5-C5-C6-O6
2	D	501	U2F	C4-C5-C6-O6
2	G	501	U2F	O5-C5-C6-O6
2	B	501	U2F	C4'-C5'-O5'-PA
2	G	501	U2F	O4'-C4'-C5'-O5'
2	A	501	U2F	PB-O3A-PA-O5'
2	E	501	U2F	PA-O3A-PB-O1
2	G	501	U2F	PA-O3A-PB-O1
2	F	501	U2F	O4'-C4'-C5'-O5'
2	E	501	U2F	C5'-O5'-PA-O2A
2	G	501	U2F	C5'-O5'-PA-O3A
2	G	501	U2F	C4'-C5'-O5'-PA
2	A	501	U2F	PA-O3A-PB-O1B
2	C	501	U2F	PA-O3A-PB-O2B
2	G	501	U2F	C3'-C4'-C5'-O5'
2	B	501	U2F	O5-C1-O1-PB
2	E	501	U2F	O5-C1-O1-PB
2	B	501	U2F	C4-C5-C6-O6
2	F	501	U2F	C3'-C4'-C5'-O5'
2	D	501	U2F	O5-C5-C6-O6
2	E	501	U2F	PB-O3A-PA-O5'
2	B	501	U2F	C1-O1-PB-O1B
2	D	501	U2F	C1-O1-PB-O1B
2	A	501	U2F	PA-O3A-PB-O2B
2	B	501	U2F	PB-O3A-PA-O2A
2	C	501	U2F	O4'-C1'-N1-C9'
2	E	501	U2F	O4'-C1'-N1-C9'
2	A	501	U2F	PB-O3A-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	501	U2F	PA-O3A-PB-O1B

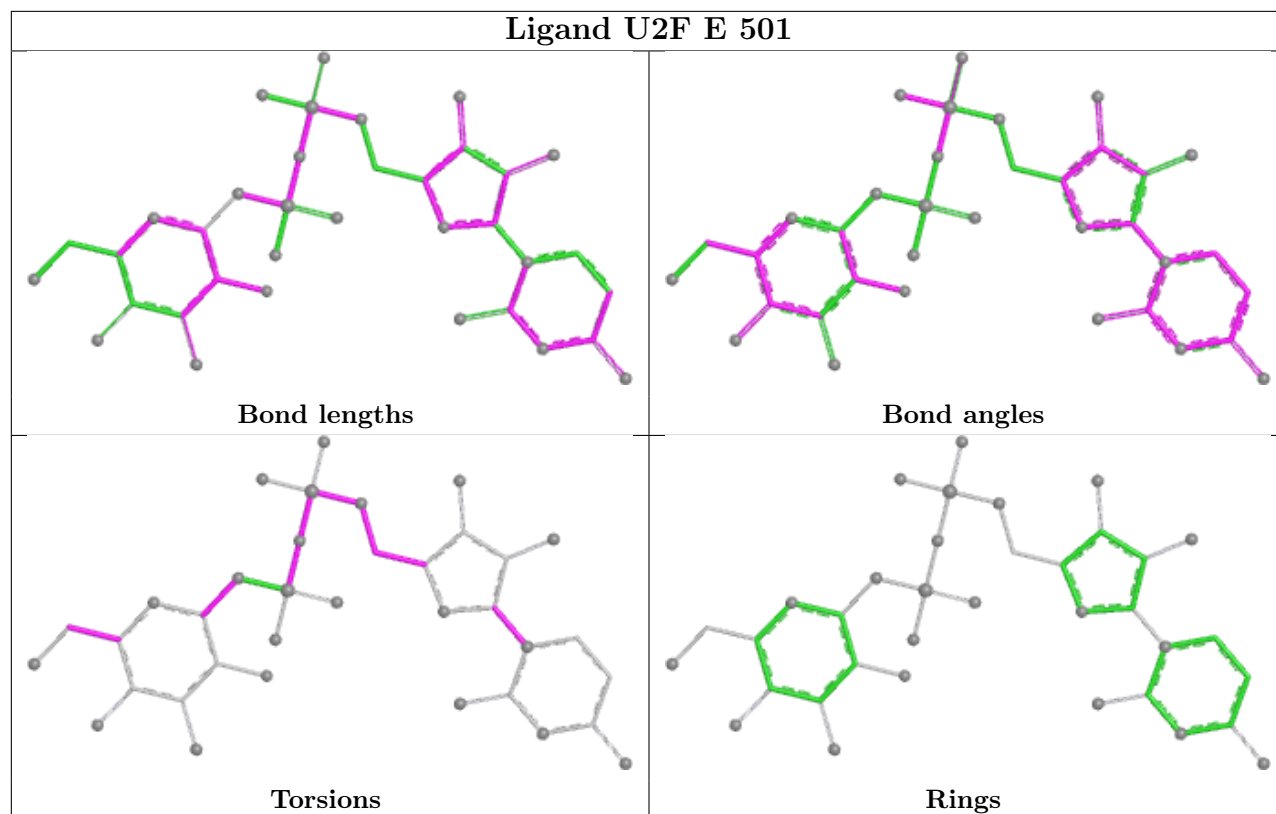
There are no ring outliers.

12 monomers are involved in 48 short contacts:

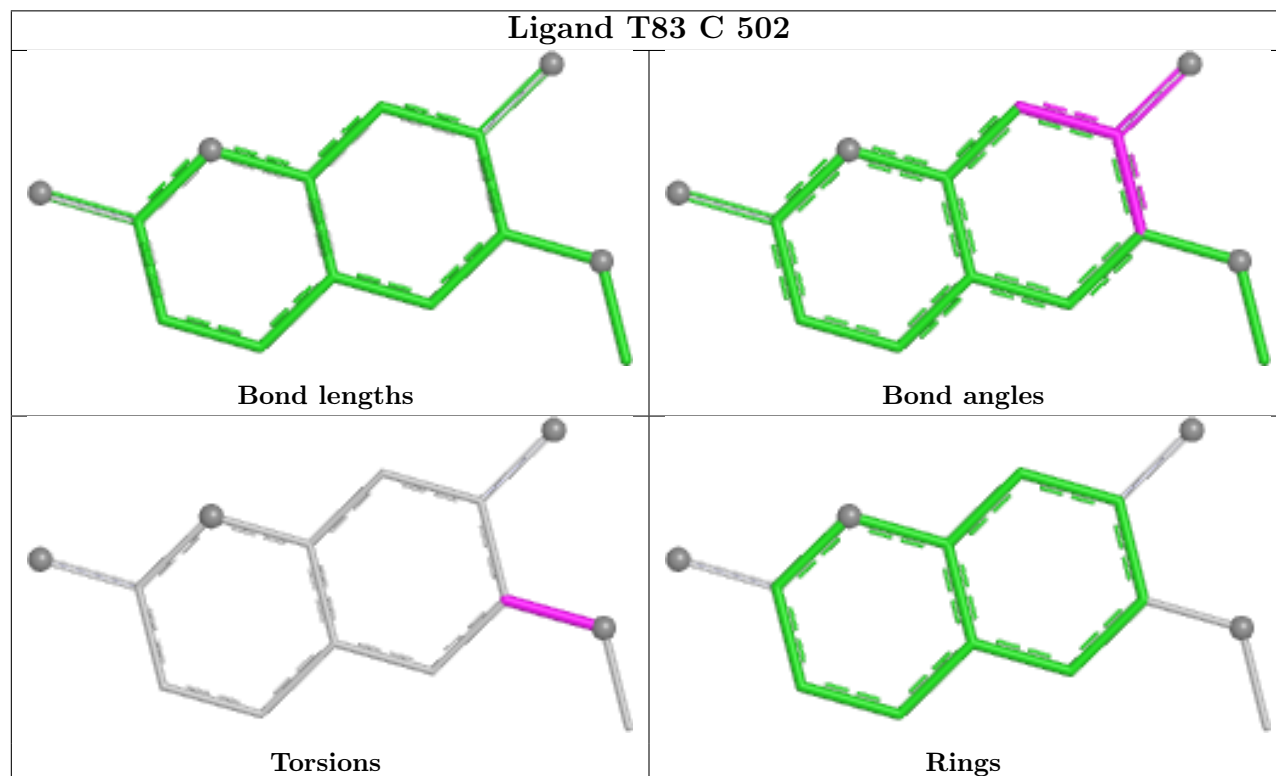
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	U2F	10	0
3	C	502	T83	1	0
2	C	501	U2F	15	0
3	B	502	T83	1	0
2	A	501	U2F	1	0
2	F	501	U2F	4	0
3	F	502	T83	1	0
2	G	501	U2F	5	0
3	D	502	T83	1	0
3	A	502	T83	2	0
2	B	501	U2F	3	0
2	D	501	U2F	5	0

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

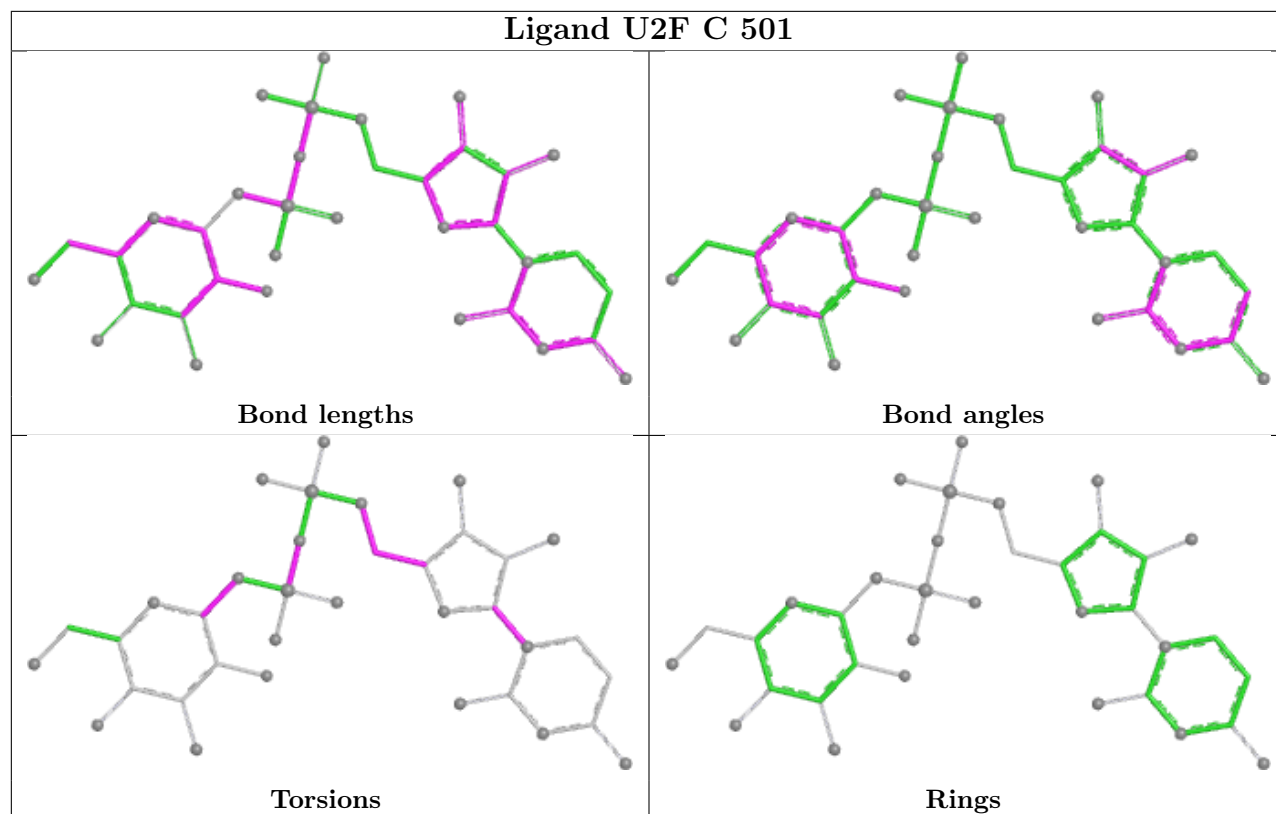
Ligand U2F E 501



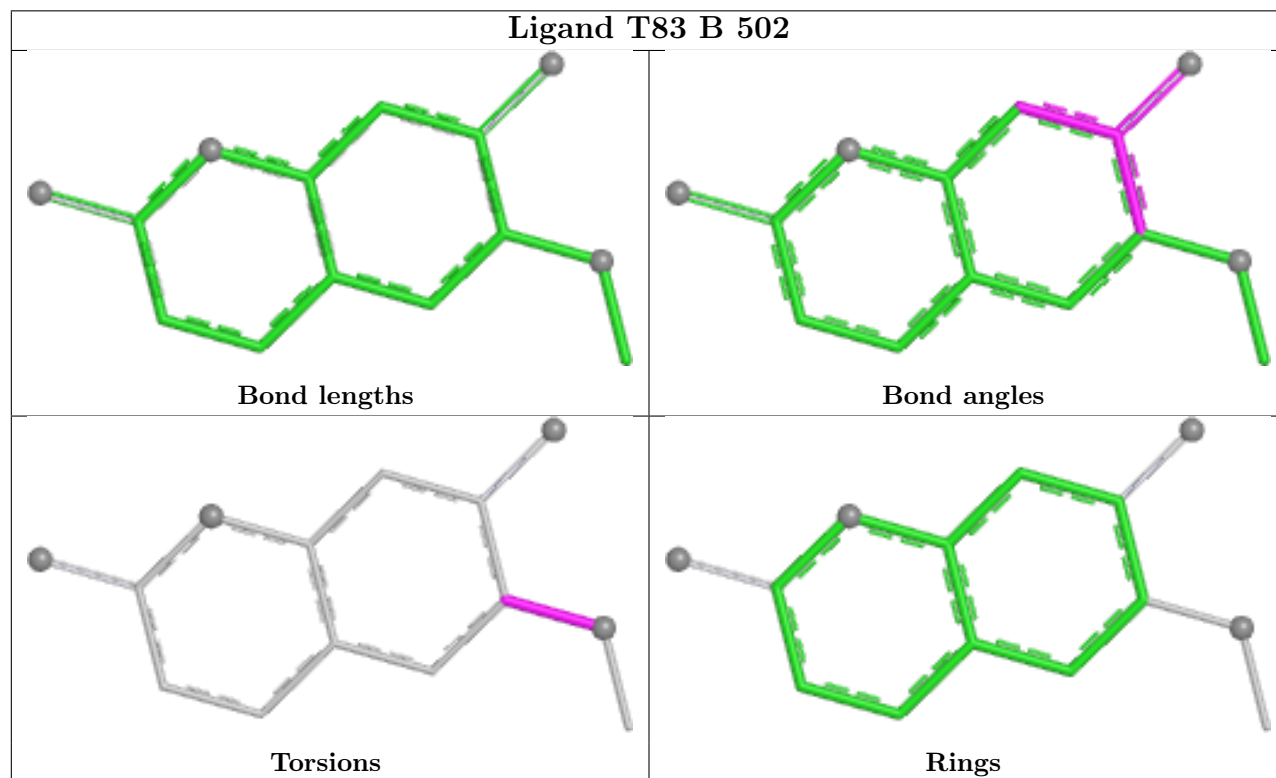
Ligand T83 C 502



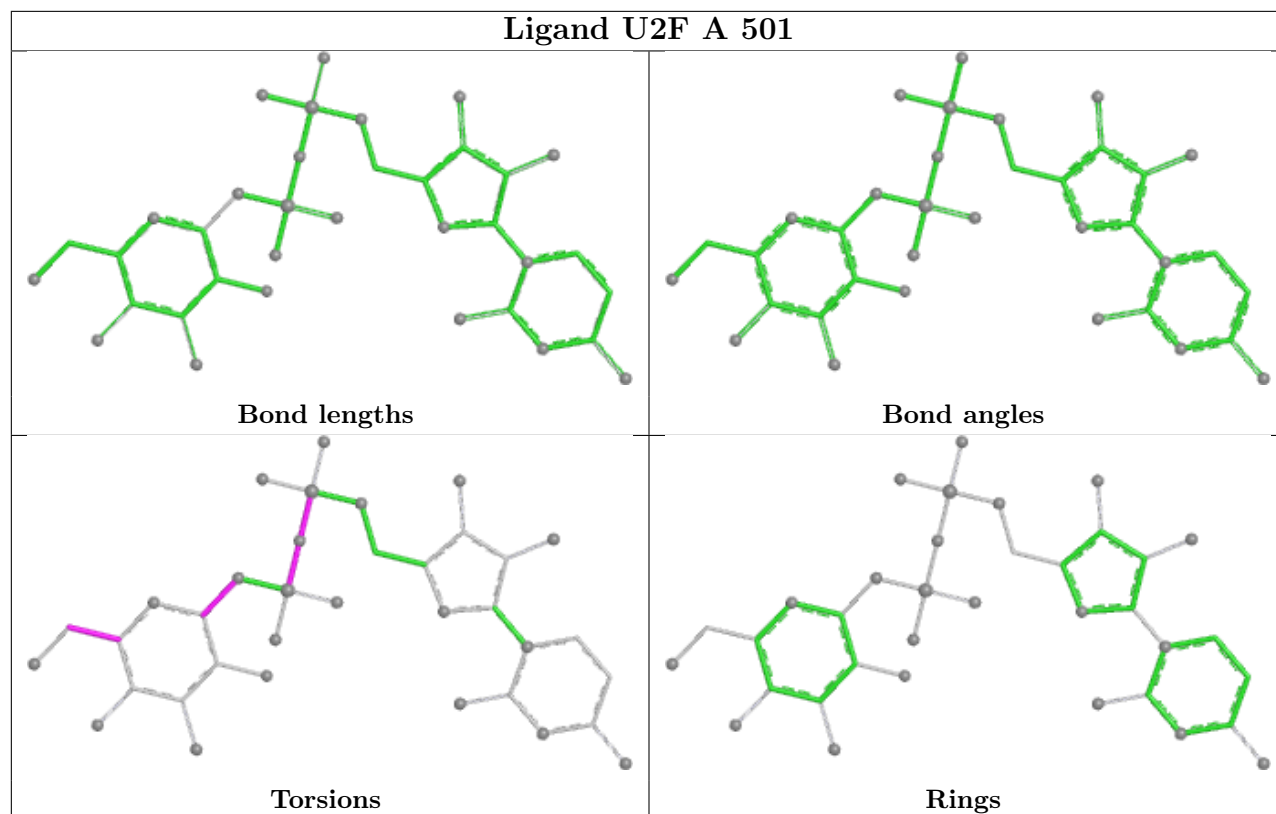
Ligand U2F C 501



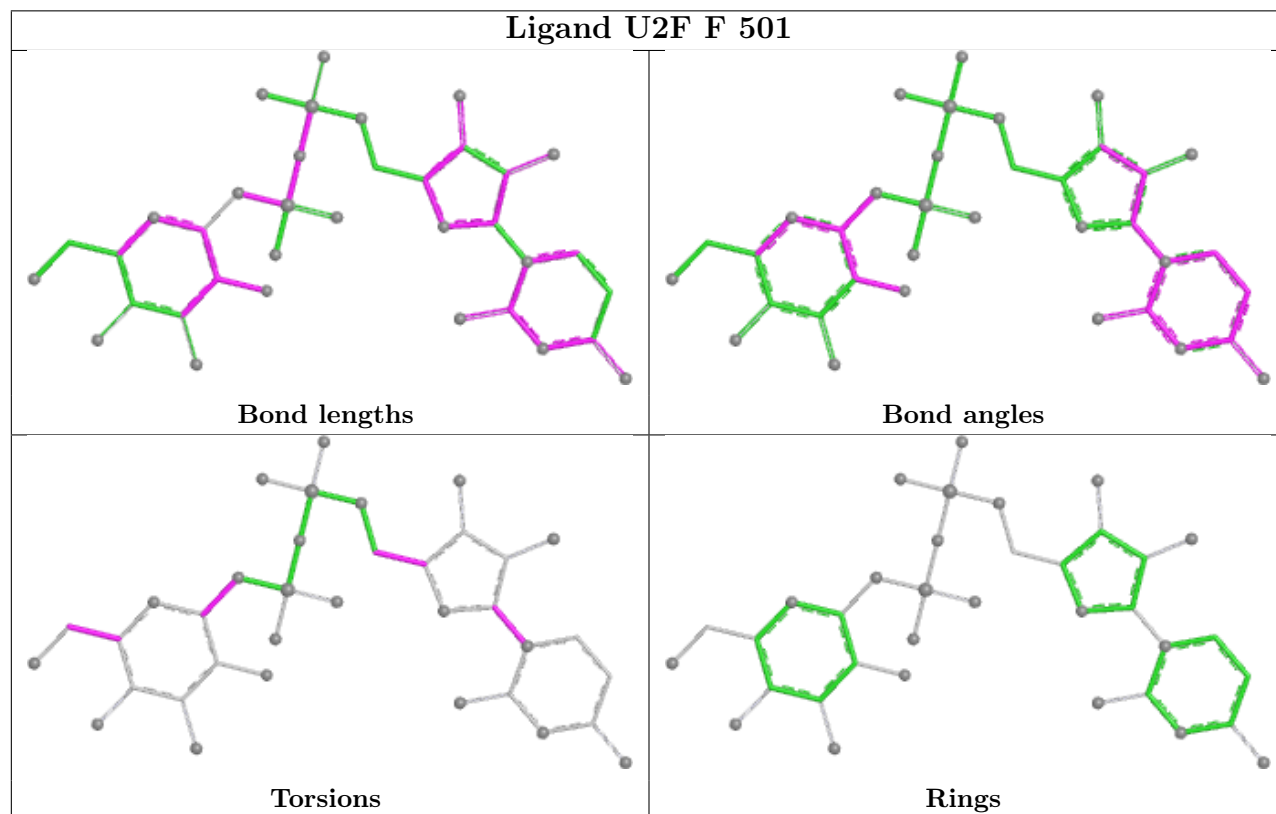
Ligand T83 B 502

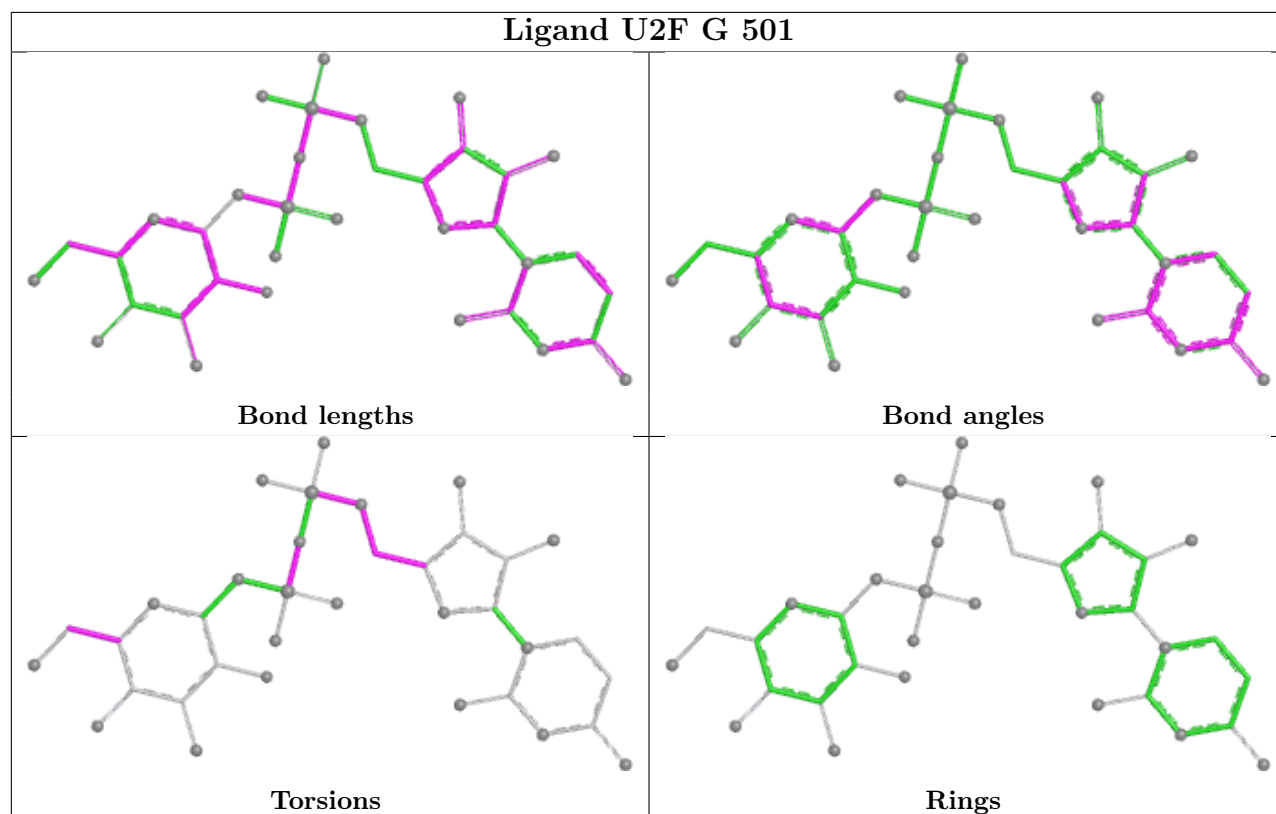
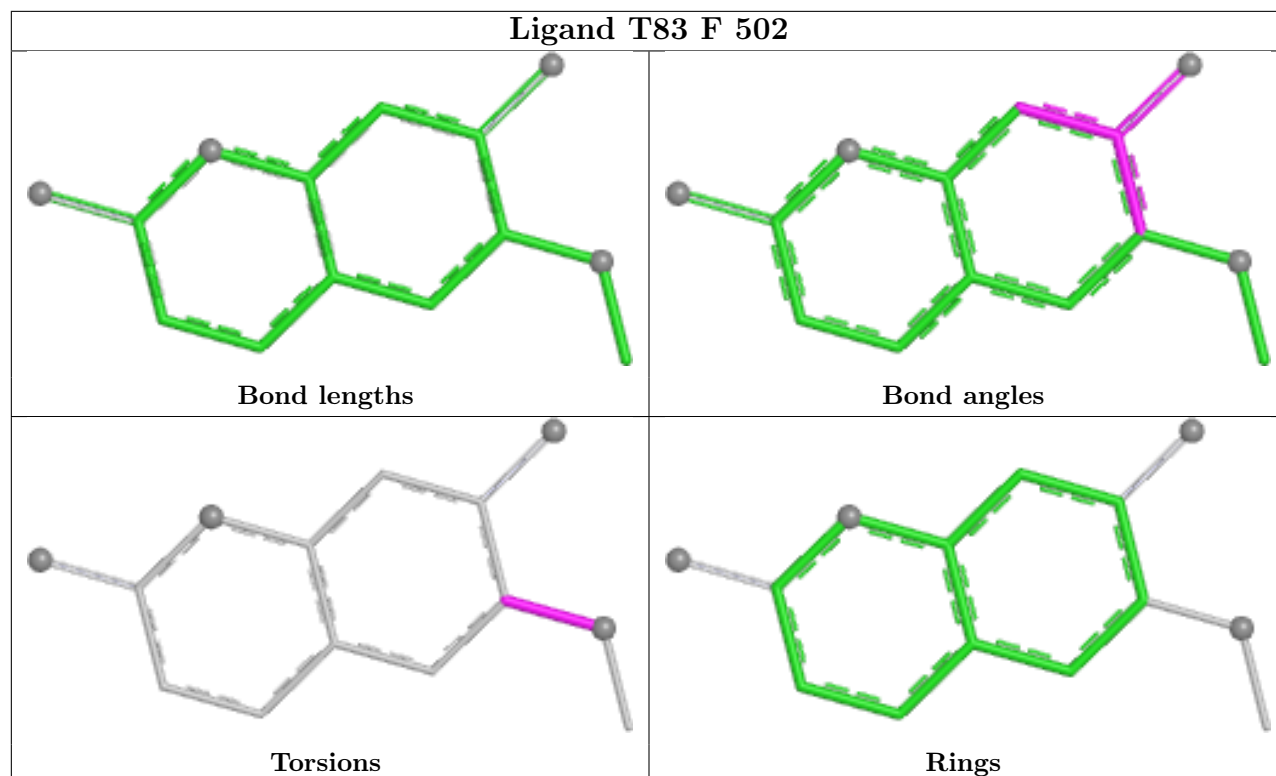


Ligand U2F A 501

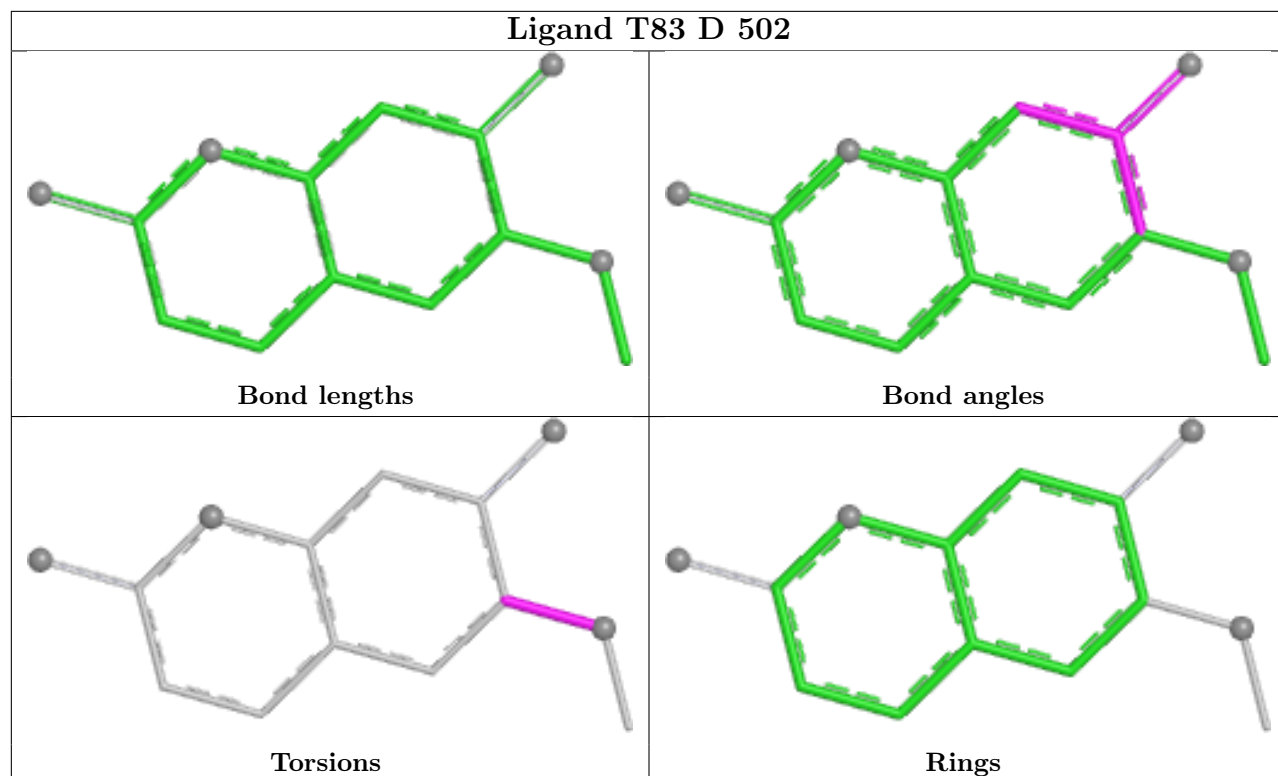


Ligand U2F F 501

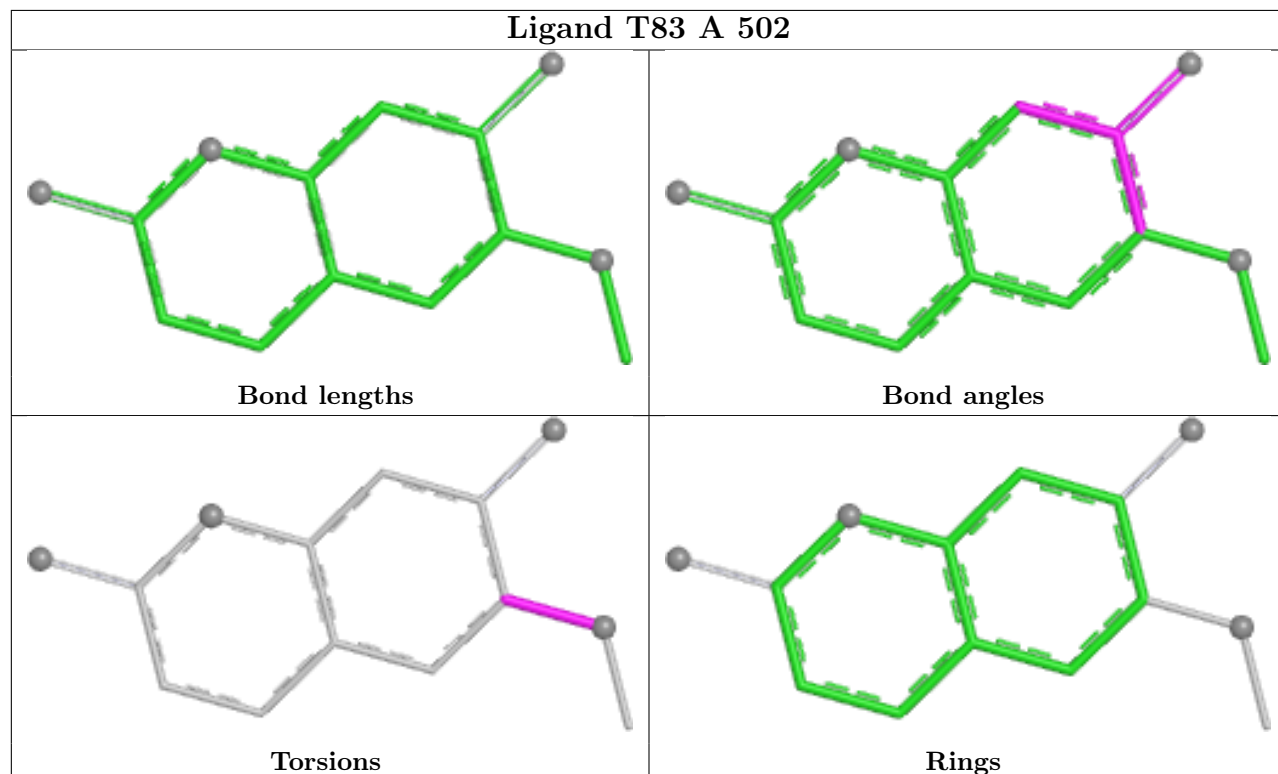




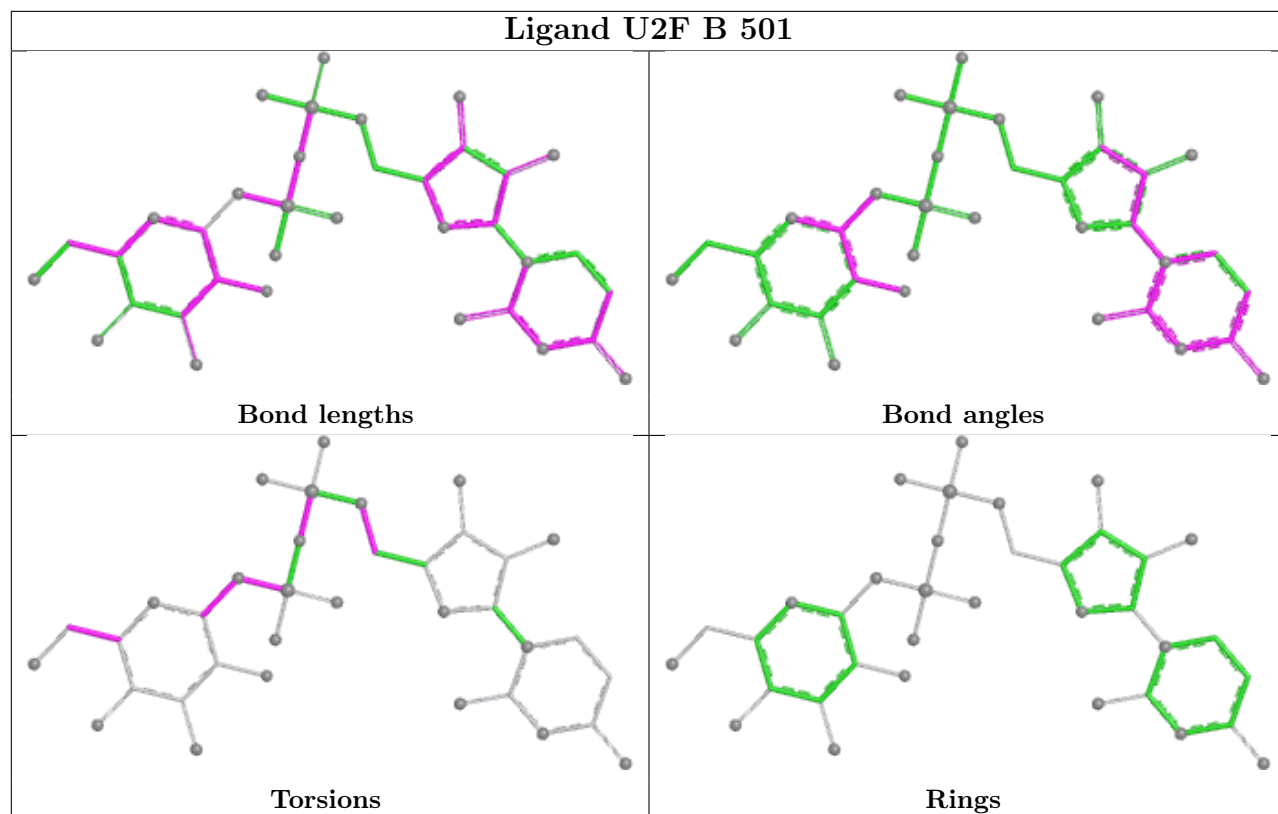
Ligand T83 D 502



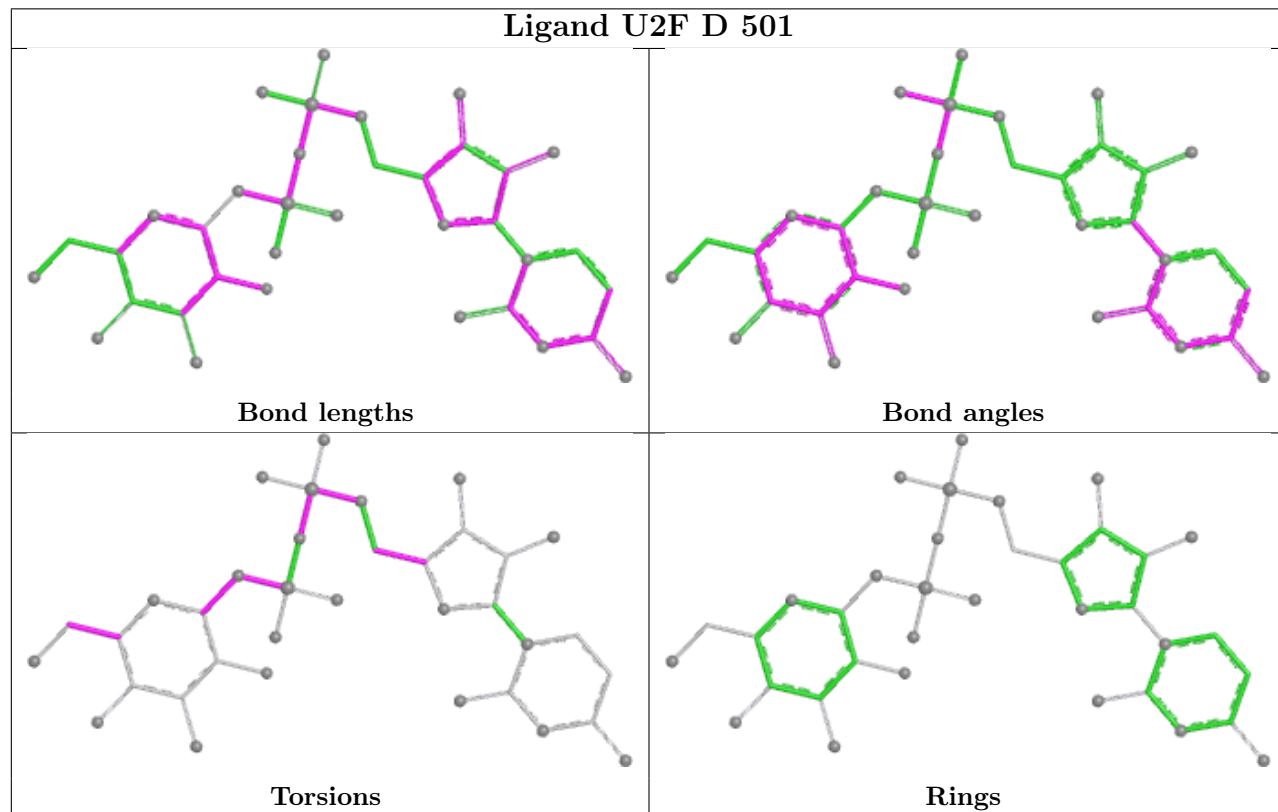
Ligand T83 A 502



Ligand U2F B 501



Ligand U2F D 501



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	455/479 (94%)	-1.52	0 100 100	11, 30, 65, 138	0
1	B	459/479 (95%)	-1.53	0 100 100	12, 28, 57, 121	0
1	C	460/479 (96%)	-1.53	0 100 100	10, 28, 61, 92	0
1	D	460/479 (96%)	-1.53	0 100 100	13, 29, 56, 97	0
1	E	459/479 (95%)	-1.51	0 100 100	10, 31, 59, 81	0
1	F	459/479 (95%)	-1.48	0 100 100	14, 34, 62, 126	0
1	G	460/479 (96%)	-1.47	0 100 100	13, 35, 67, 94	0
All	All	3212/3353 (95%)	-1.51	0 100 100	10, 30, 61, 138	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

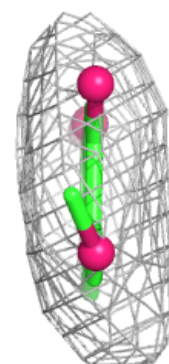
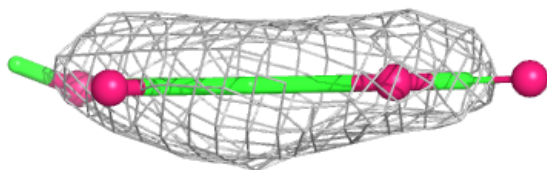
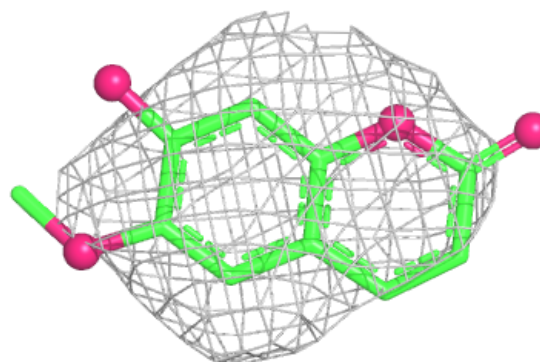
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	T83	F	502	14/14	0.98	0.05	62,68,75,76	0
2	U2F	G	501	36/36	0.99	0.04	36,63,119,125	0
3	T83	A	502	14/14	0.99	0.04	52,62,85,95	0
3	T83	B	502	14/14	0.99	0.04	49,54,62,66	0
3	T83	C	502	14/14	0.99	0.04	56,67,80,83	0
3	T83	D	502	14/14	0.99	0.04	35,56,75,87	0
2	U2F	F	501	36/36	0.99	0.03	33,49,79,80	0
2	U2F	C	501	36/36	1.00	0.03	30,69,117,141	0
2	U2F	D	501	36/36	1.00	0.03	34,49,69,84	0
2	U2F	E	501	36/36	1.00	0.03	39,65,105,117	0
2	U2F	A	501	36/36	1.00	0.02	29,38,78,92	0
2	U2F	B	501	36/36	1.00	0.03	22,27,60,62	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.

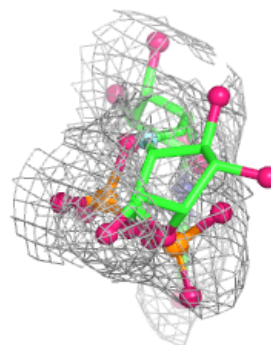
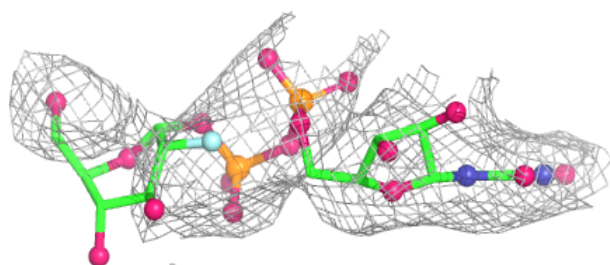
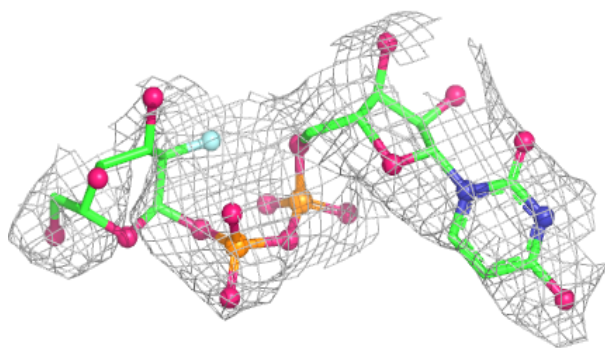
Electron density around T83 F 502:

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

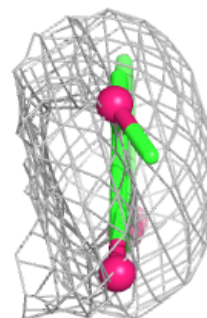
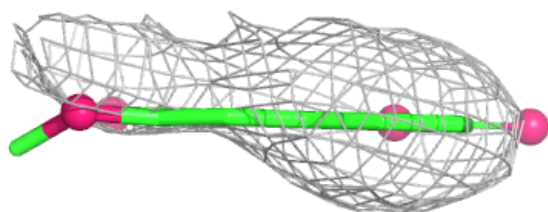
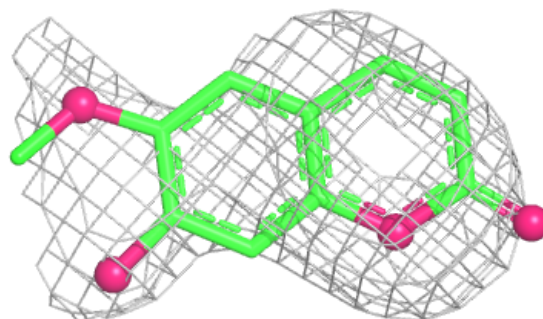


Electron density around U2F G 501:

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

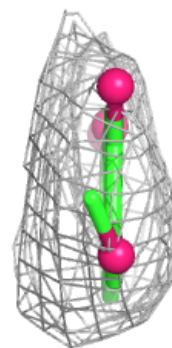
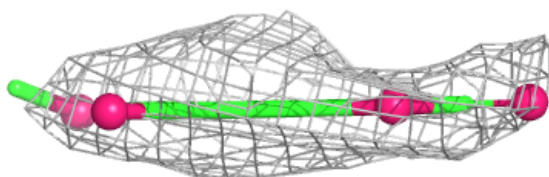
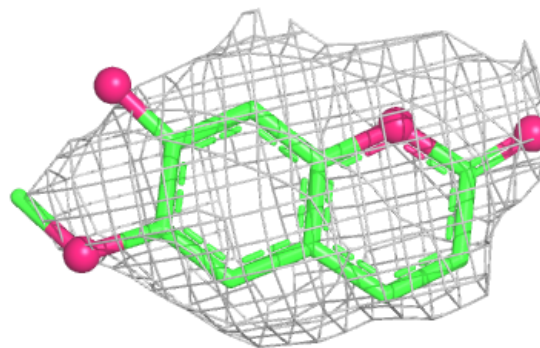
**Electron density around T83 A 502:**

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

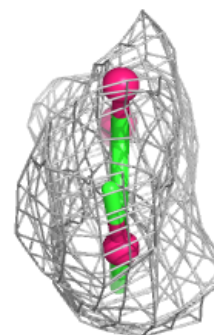
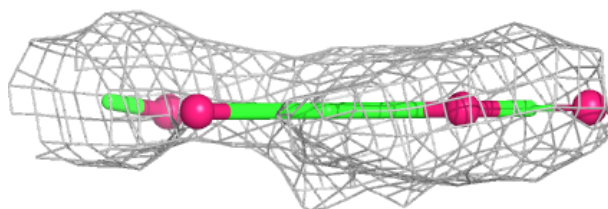
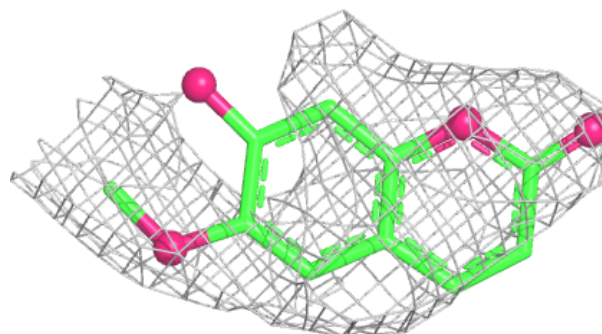


Electron density around T83 B 502:

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

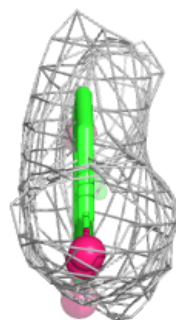
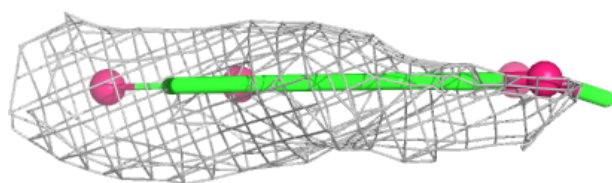
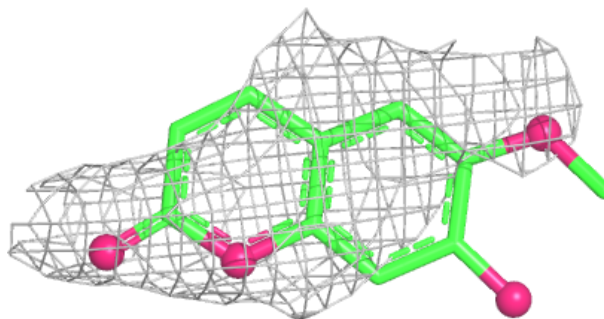
**Electron density around T83 C 502:**

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

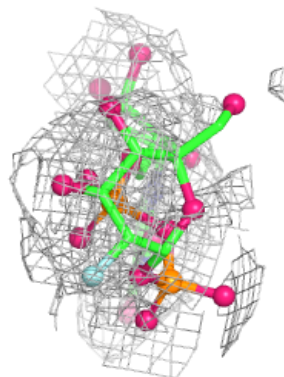
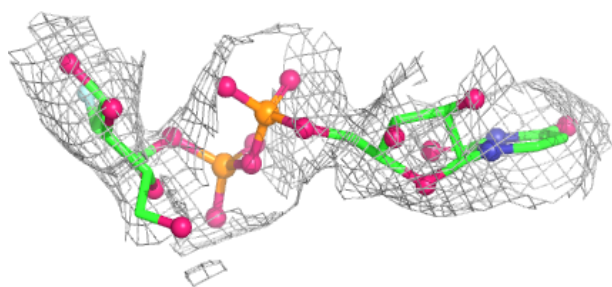
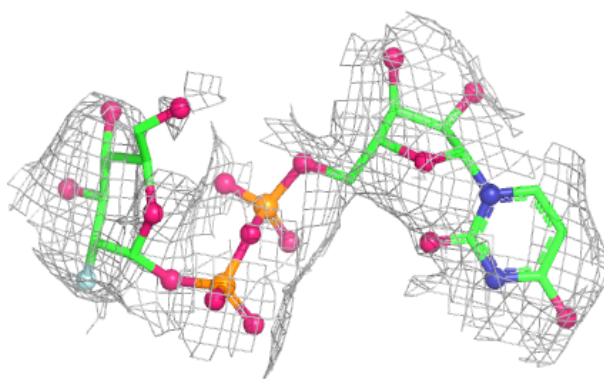


Electron density around T83 D 502:

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

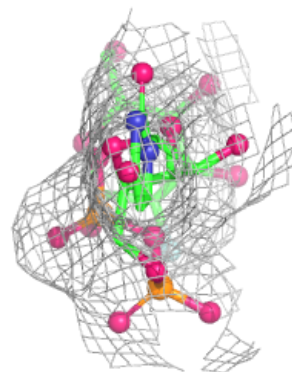
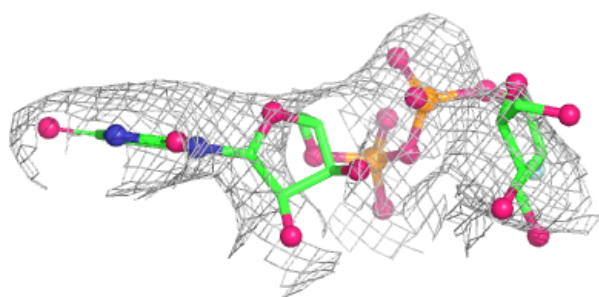
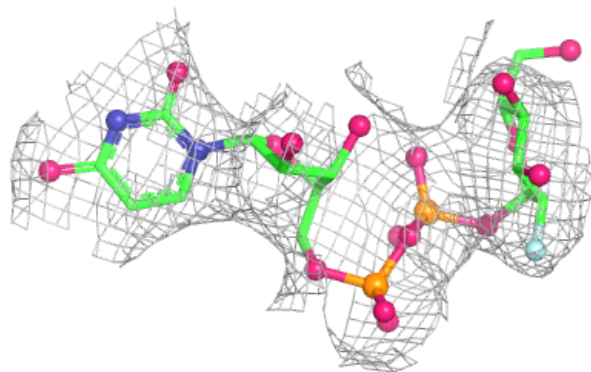
**Electron density around U2F F 501:**

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

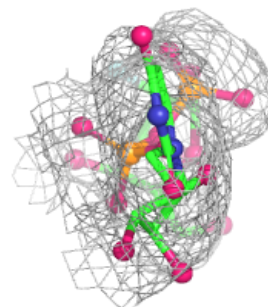
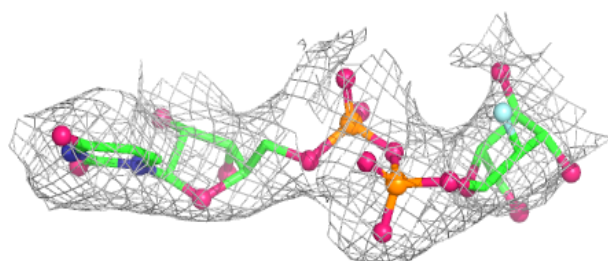
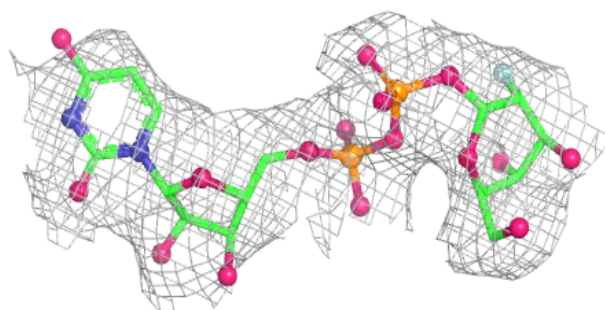


Electron density around U2F C 501:

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

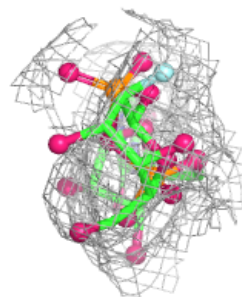
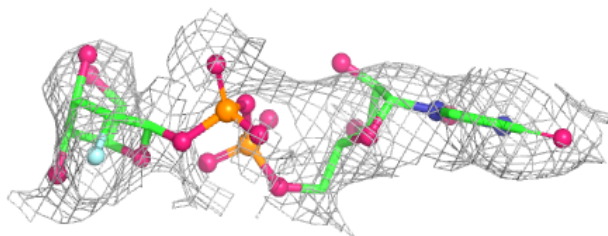
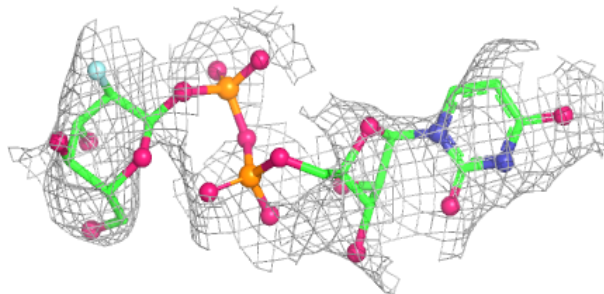
**Electron density around U2F D 501:**

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

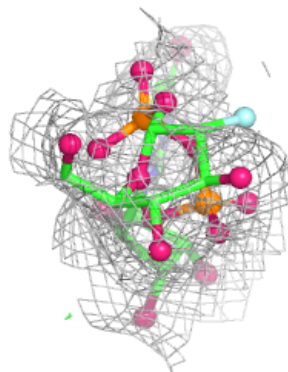
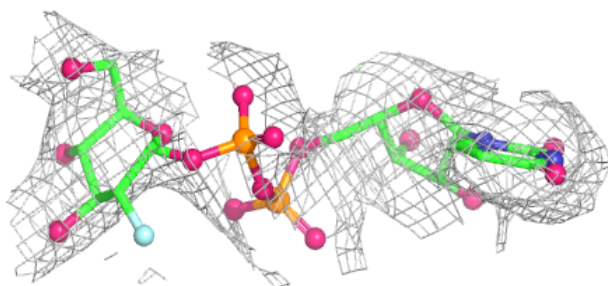
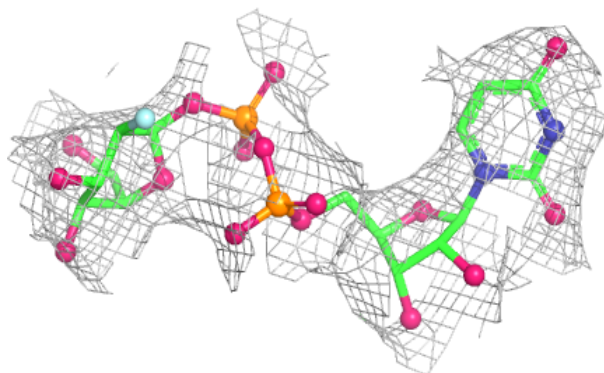


Electron density around U2F E 501:

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

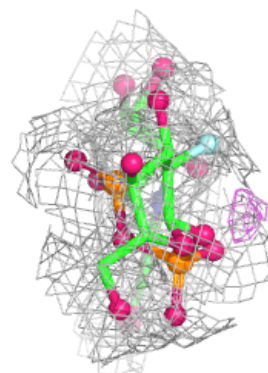
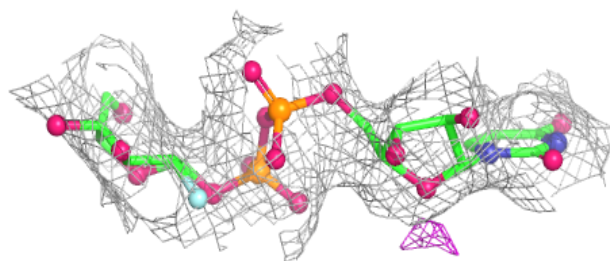
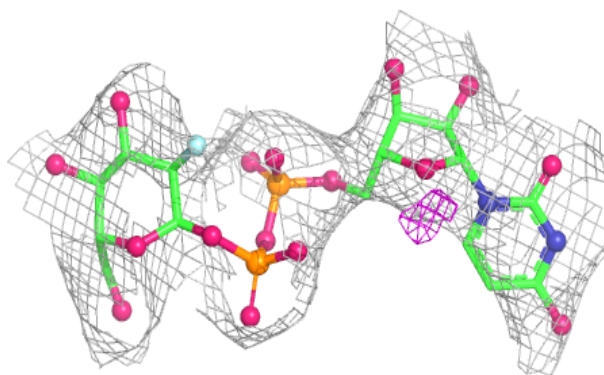
**Electron density around U2F A 501:**

$2mF_o-DF_c$ (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.