



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 12:05 PM UTC

PDB ID : 1Z7E / pdb_00001z7e
Title : Crystal structure of full length ArnA
Authors : Gatzeva-Topalova, P.Z.; May, A.P.; Sousa, M.C.
Deposited on : 2005-03-24
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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

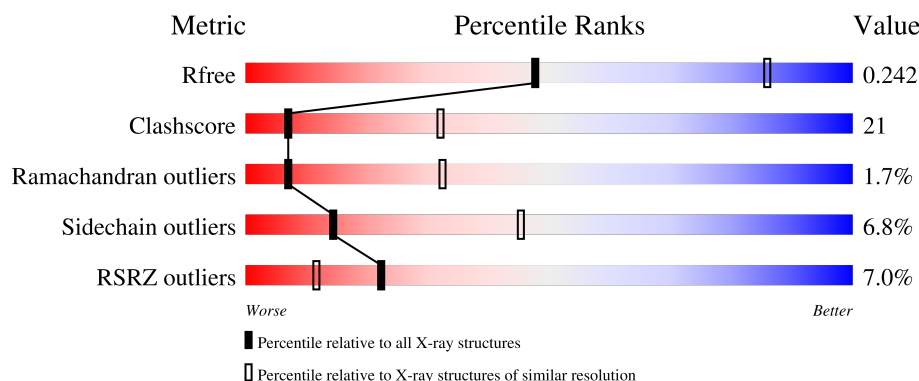
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	660	5% 56% 36% 5%
1	B	660	7% 57% 34% 5%
1	C	660	6% 58% 34% 5%
1	D	660	6% 57% 35% 5%
1	E	660	4% 58% 34% 5%

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Mol	Chain	Length	Quality of chain
1	F	660	14% 55% 37%

2 Entry composition [i](#)

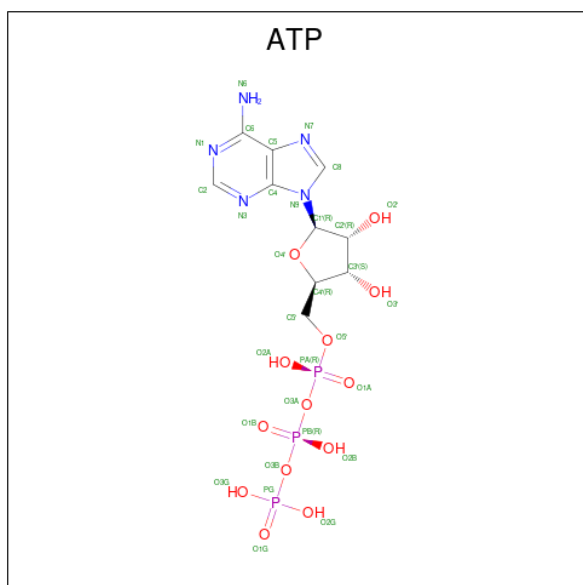
There are 3 unique types of molecules in this entry. The entry contains 30556 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 protein ArnA.

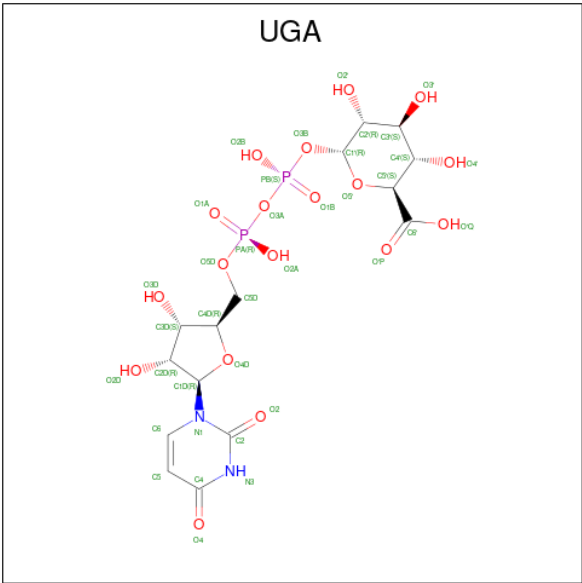
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	B	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	C	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	D	644	Total	C	N	O	S	0	0	0
			5048	3227	888	914	19			
1	E	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			
1	F	639	Total	C	N	O	S	0	0	0
			5020	3210	883	908	19			

- Molecule 2 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	E	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
2	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 3 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (CCD ID: UGA) (formula: C₁₅H₂₂N₂O₁₈P₂).

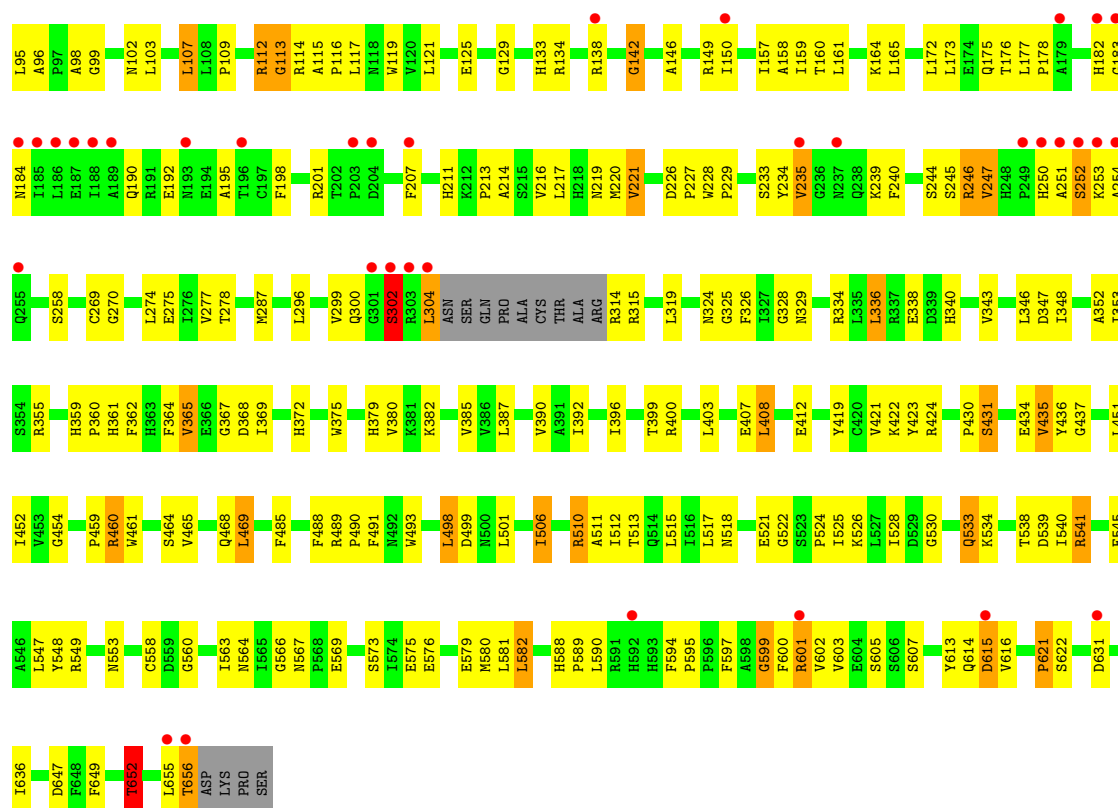


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	B	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	C	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	D	1	Total	C	N	O	P	0	0
			37	15	2	18	2		
3	E	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

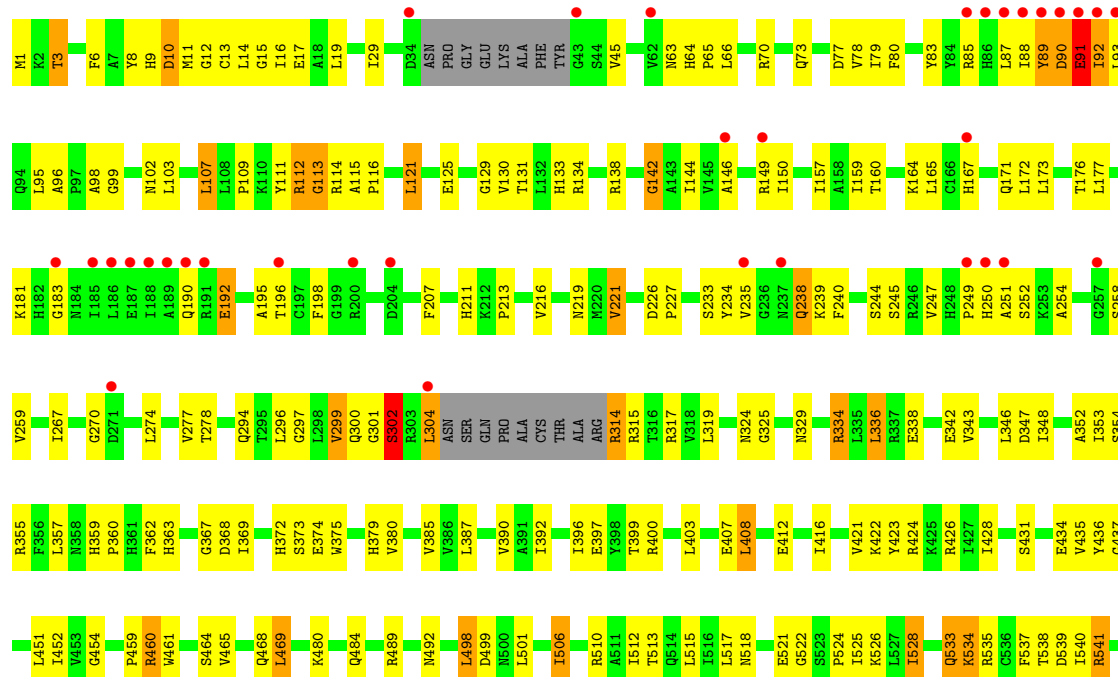
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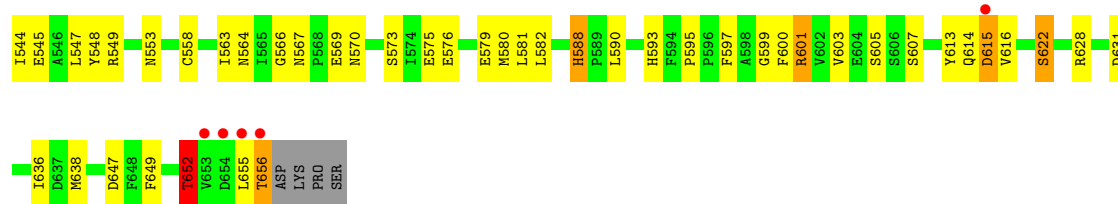
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	F	1	Total	C	N	O	P	0	0
			37	15	2	18	2		

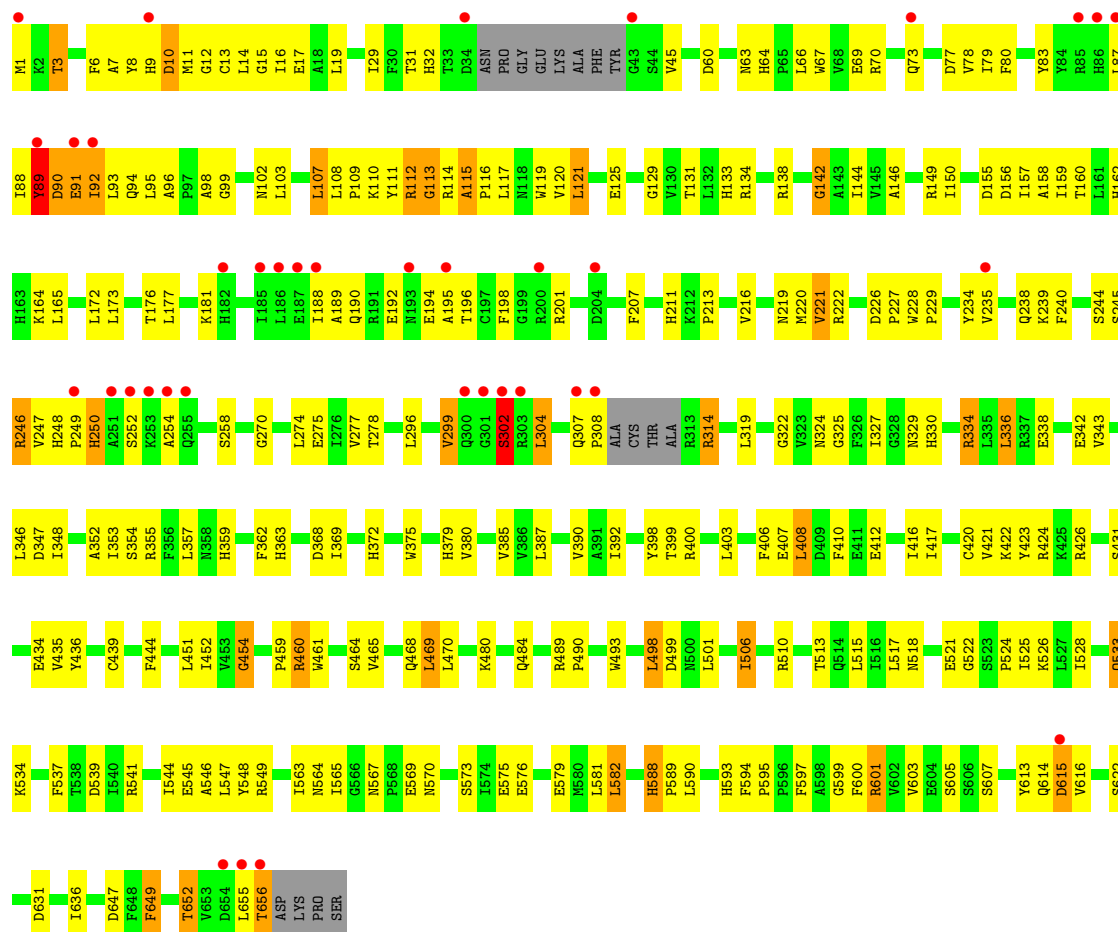


• Molecule 1: protein ArnA

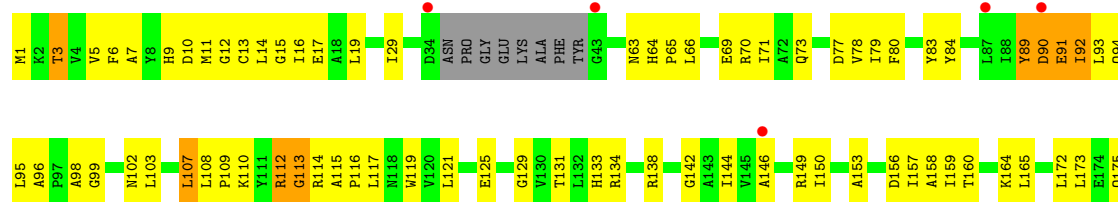


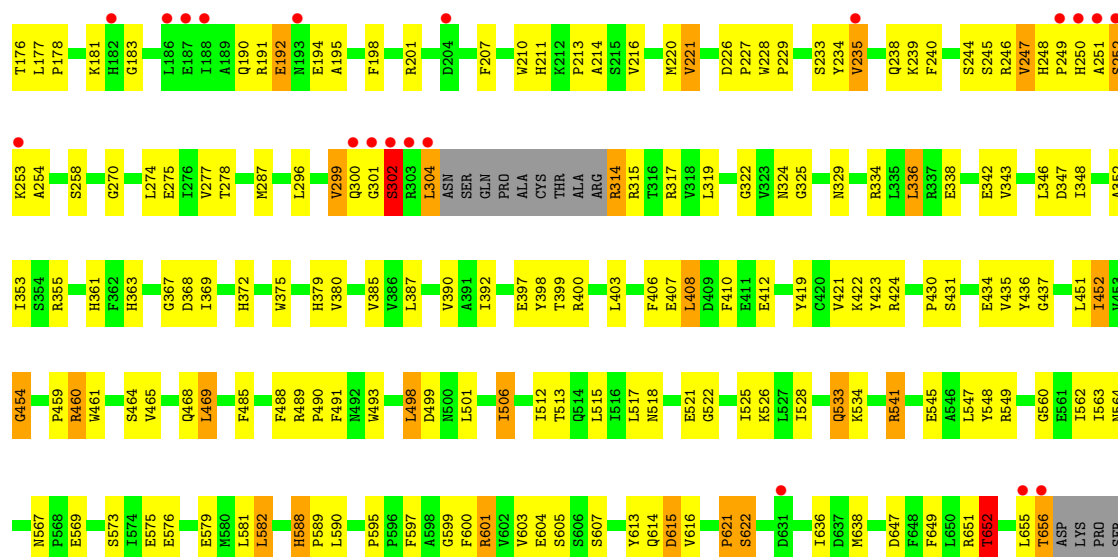


• Molecule 1: protein ArnA

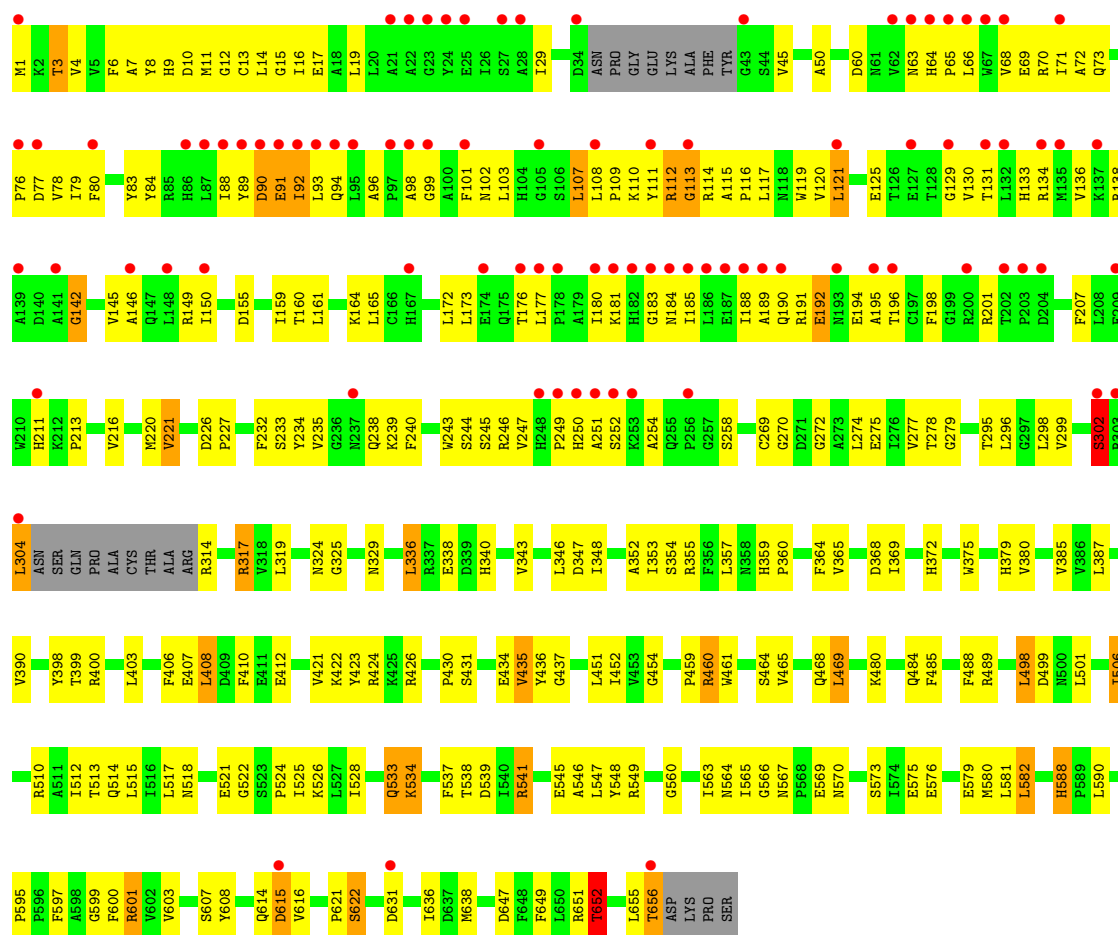


• Molecule 1: protein ArnA





• Molecule 1: protein ArnA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.69Å 166.23Å 261.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-3.00) 95.2 (50.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.77 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.247 0.222 , 0.242	Depositor DCC
R_{free} test set	12667 reflections (9.56%)	wwPDB-VP
Wilson B-factor (Å ²)	47.0	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	30556	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: ATP, UGA

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	0.50	0/5143	0.97	21/6992 (0.3%)
1	B	0.52	0/5143	0.97	18/6992 (0.3%)
1	C	0.53	0/5143	0.98	19/6992 (0.3%)
1	D	0.50	0/5172	0.98	21/7033 (0.3%)
1	E	0.49	0/5143	0.97	21/6992 (0.3%)
1	F	0.52	0/5143	0.96	15/6992 (0.2%)
All	All	0.51	0/30887	0.97	115/41993 (0.3%)

There are no bond length outliers.

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	380	VAL	N-CA-C	-8.57	102.07	110.72
1	A	380	VAL	N-CA-C	-8.53	102.11	110.72
1	F	380	VAL	N-CA-C	-8.21	102.42	110.72
1	C	380	VAL	N-CA-C	-8.19	102.45	110.72
1	B	380	VAL	N-CA-C	-7.75	102.89	110.72
1	D	622	SER	N-CA-C	-7.29	97.37	109.46
1	E	622	SER	N-CA-C	-7.26	97.41	109.46
1	B	652	THR	N-CA-C	-7.11	104.87	113.97
1	E	380	VAL	N-CA-C	-7.06	103.59	110.72
1	A	622	SER	N-CA-C	-7.00	97.84	109.46
1	C	622	SER	N-CA-C	-6.93	97.95	109.46
1	F	622	SER	N-CA-C	-6.78	98.21	109.46
1	D	3	THR	N-CA-C	6.66	119.29	109.24
1	F	3	THR	N-CA-C	6.57	119.16	109.24
1	D	299	VAL	N-CA-C	-6.55	95.71	109.34
1	D	563	ILE	N-CA-C	6.49	117.37	107.77
1	E	562	ILE	N-CA-C	-6.48	99.04	108.11
1	D	631	ASP	N-CA-C	-6.36	103.16	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	VAL	N-CA-C	6.30	116.93	107.80
1	A	563	ILE	N-CA-C	6.29	117.08	107.77
1	C	299	VAL	N-CA-C	-6.27	96.30	109.34
1	C	249	PRO	N-CA-C	-6.25	106.35	114.03
1	F	615	ASP	N-CA-C	6.21	118.00	109.18
1	B	622	SER	N-CA-C	-6.21	99.15	109.46
1	F	652	THR	N-CA-C	-6.18	105.90	113.50
1	E	652	THR	N-CA-C	-6.17	105.92	113.50
1	E	302	SER	N-CA-C	6.14	123.88	110.80
1	D	588	HIS	N-CA-C	6.08	117.55	109.83
1	C	588	HIS	N-CA-C	6.07	117.35	109.64
1	F	638	MET	N-CA-C	6.04	118.35	111.11
1	B	328	GLY	N-CA-C	6.03	119.93	112.64
1	C	631	ASP	N-CA-C	-6.02	103.62	111.74
1	A	3	THR	N-CA-C	6.00	118.07	109.14
1	E	299	VAL	N-CA-C	-5.99	96.88	109.34
1	D	302	SER	N-CA-C	5.99	123.55	110.80
1	A	238	GLN	N-CA-C	5.98	119.27	109.76
1	F	249	PRO	N-CA-C	-5.97	106.68	114.03
1	B	419	TYR	N-CA-C	-5.97	104.78	111.28
1	F	563	ILE	N-CA-C	5.96	116.59	107.77
1	A	299	VAL	N-CA-C	-5.95	96.96	109.34
1	C	652	THR	N-CA-C	-5.93	106.59	113.88
1	F	299	VAL	N-CA-C	-5.87	97.14	109.34
1	D	249	PRO	N-CA-C	-5.83	106.47	113.98
1	B	299	VAL	N-CA-C	-5.81	97.25	109.34
1	E	3	THR	N-CA-C	5.77	117.95	109.24
1	E	249	PRO	N-CA-C	-5.74	106.97	114.03
1	F	238	GLN	N-CA-C	5.73	118.87	109.76
1	C	343	VAL	N-CA-C	5.71	116.07	107.80
1	B	563	ILE	N-CA-C	5.70	116.21	107.77
1	B	302	SER	N-CA-C	5.69	122.92	110.80
1	C	85	ARG	N-CA-C	5.68	118.33	111.40
1	C	563	ILE	N-CA-C	5.65	116.13	107.77
1	B	631	ASP	N-CA-C	-5.64	103.62	111.52
1	E	89	TYR	N-CA-C	5.63	118.73	109.72
1	C	615	ASP	N-CA-C	5.59	117.12	109.18
1	C	238	GLN	N-CA-C	5.57	118.61	109.76
1	E	343	VAL	N-CA-C	5.56	116.11	107.99
1	E	235	VAL	N-CA-C	-5.56	97.88	106.72
1	A	85	ARG	N-CA-C	5.54	118.16	111.40
1	A	442	LYS	N-CA-C	-5.53	105.33	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	THR	N-CA-C	5.53	117.59	109.24
1	A	302	SER	N-CA-C	5.50	122.52	110.80
1	D	238	GLN	N-CA-C	5.46	118.44	109.76
1	A	615	ASP	N-CA-C	5.44	116.91	109.18
1	C	302	SER	N-CA-C	5.44	122.39	110.80
1	D	10	ASP	N-CA-C	5.43	117.64	111.02
1	E	322	GLY	N-CA-C	-5.43	106.18	115.08
1	D	322	GLY	N-CA-C	-5.42	106.19	115.08
1	A	89	TYR	N-CA-C	5.42	118.39	109.72
1	B	615	ASP	N-CA-C	5.41	116.87	109.18
1	A	419	TYR	N-CA-C	-5.41	105.38	111.28
1	F	631	ASP	N-CA-C	-5.41	104.44	111.74
1	F	302	SER	N-CA-C	5.39	122.28	110.80
1	A	599	GLY	N-CA-C	5.38	119.64	112.65
1	A	652	THR	N-CA-C	-5.37	106.89	113.50
1	A	249	PRO	N-CA-C	-5.37	107.06	113.98
1	A	631	ASP	N-CA-C	-5.36	104.50	111.74
1	B	599	GLY	N-CA-C	5.31	119.55	112.65
1	E	588	HIS	N-CA-C	5.29	116.55	109.83
1	D	454	GLY	CA-C-N	5.28	125.57	119.92
1	D	454	GLY	C-N-CA	5.28	125.57	119.92
1	E	615	ASP	N-CA-C	5.27	116.30	108.86
1	C	3	THR	N-CA-C	5.27	116.99	109.14
1	A	343	VAL	N-CA-C	5.26	115.43	107.80
1	C	89	TYR	N-CA-C	5.25	118.11	109.72
1	F	343	VAL	N-CA-C	5.22	115.61	107.99
1	C	638	MET	N-CA-C	5.22	117.37	111.11
1	E	419	TYR	N-CA-C	-5.21	105.60	111.28
1	D	343	VAL	N-CA-C	5.16	115.53	107.99
1	E	84	TYR	N-CA-C	-5.15	102.66	110.28
1	F	588	HIS	CA-C-N	5.15	125.19	119.32
1	F	588	HIS	C-N-CA	5.15	125.19	119.32
1	D	87	LEU	N-CA-C	5.14	117.11	108.73
1	B	89	TYR	N-CA-C	5.13	117.60	109.50
1	B	5	VAL	N-CA-C	5.12	115.96	108.53
1	C	10	ASP	N-CA-C	5.12	117.27	111.02
1	A	322	GLY	N-CA-C	-5.11	106.71	115.08
1	B	382	LYS	N-CA-C	5.09	118.64	112.23
1	C	628	ARG	N-CA-C	5.09	116.52	111.07
1	E	452	ILE	N-CA-C	5.09	115.18	107.75
1	E	563	ILE	N-CA-C	5.05	115.24	107.77
1	E	454	GLY	CA-C-N	5.04	125.31	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	454	GLY	C-N-CA	5.04	125.31	119.92
1	D	89	TYR	N-CA-C	5.04	117.78	109.72
1	A	577	LEU	N-CA-C	-5.03	105.80	111.28
1	D	649	PHE	N-CA-C	5.02	116.76	111.28
1	B	235	VAL	N-CA-C	-5.02	98.90	109.34
1	D	359	HIS	CA-C-N	5.02	124.80	119.28
1	D	359	HIS	C-N-CA	5.02	124.80	119.28
1	D	615	ASP	N-CA-C	5.01	116.30	109.18
1	A	433	SER	N-CA-C	-5.00	107.12	113.18
1	E	638	MET	N-CA-C	5.00	117.11	111.11
1	A	372	HIS	N-CA-C	5.00	117.34	109.39
1	B	85	ARG	N-CA-C	5.00	117.50	111.40
1	C	428	ILE	N-CA-C	-5.00	99.75	106.85

There are no chirality outliers.

There are no planarity outliers.

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	5020	0	4924	218	0
1	B	5020	0	4924	214	2
1	C	5020	0	4924	210	2
1	D	5048	0	4942	209	0
1	E	5020	0	4924	215	0
1	F	5020	0	4924	226	0
2	A	31	0	12	5	0
2	B	31	0	12	4	0
2	C	31	0	12	4	0
2	D	31	0	12	4	0
2	E	31	0	12	2	0
2	F	31	0	12	3	0
3	A	37	0	19	1	0
3	B	37	0	19	1	0
3	C	37	0	19	1	0
3	D	37	0	19	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	37	0	19	1	0
3	F	37	0	19	1	0
All	All	30556	0	29748	1266	2

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 (1266) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:533:GLN:H	1:E:533:GLN:NE2	1.56	1.03
1:A:533:GLN:H	1:A:533:GLN:NE2	1.58	1.01
1:C:533:GLN:H	1:C:533:GLN:NE2	1.59	1.00
1:F:533:GLN:H	1:F:533:GLN:NE2	1.61	0.97
1:D:533:GLN:H	1:D:533:GLN:NE2	1.61	0.97
1:B:533:GLN:NE2	1:B:533:GLN:H	1.61	0.96
1:D:112:ARG:HH12	1:D:190:GLN:HE22	1.04	0.96
1:D:368:ASP:H	1:D:372:HIS:HD2	1.05	0.96
1:C:112:ARG:HH12	1:C:190:GLN:HE22	0.96	0.96
1:D:533:GLN:H	1:D:533:GLN:HE21	0.96	0.95
1:B:112:ARG:NH1	1:B:190:GLN:HE22	1.65	0.94
1:C:368:ASP:H	1:C:372:HIS:HD2	1.14	0.93
1:F:112:ARG:HH12	1:F:190:GLN:HE22	1.02	0.93
1:A:112:ARG:HH12	1:A:190:GLN:HE22	0.98	0.92
1:E:533:GLN:HE21	1:E:533:GLN:N	1.67	0.91
1:A:368:ASP:H	1:A:372:HIS:HD2	1.17	0.91
1:E:112:ARG:NH1	1:E:190:GLN:HE22	1.68	0.91
1:B:112:ARG:HH12	1:B:190:GLN:NE2	1.68	0.90
1:A:13:CYS:O	1:A:17:GLU:HG3	1.71	0.90
1:C:533:GLN:HE21	1:C:533:GLN:N	1.69	0.90
1:B:533:GLN:H	1:B:533:GLN:HE21	0.90	0.90
1:A:533:GLN:HE21	1:A:533:GLN:N	1.67	0.90
1:B:533:GLN:HE21	1:B:533:GLN:N	1.70	0.90
1:F:368:ASP:H	1:F:372:HIS:HD2	1.13	0.90
1:B:368:ASP:H	1:B:372:HIS:HD2	1.15	0.89
1:F:13:CYS:O	1:F:17:GLU:HG3	1.73	0.89
1:F:533:GLN:H	1:F:533:GLN:HE21	0.93	0.89
1:C:533:GLN:H	1:C:533:GLN:HE21	0.92	0.89
1:F:1:MET:HE2	1:F:77:ASP:HB3	1.55	0.88
1:E:533:GLN:H	1:E:533:GLN:HE21	0.88	0.88
1:E:368:ASP:H	1:E:372:HIS:HD2	1.15	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HA	1:B:518:ASN:HD22	1.37	0.88
1:C:588:HIS:CD2	1:C:590:LEU:H	1.92	0.88
1:C:258:SER:HA	1:C:302:SER:HA	1.56	0.87
1:C:515:LEU:HA	1:C:518:ASN:HD22	1.40	0.87
1:F:533:GLN:HE21	1:F:533:GLN:N	1.73	0.87
1:E:515:LEU:HA	1:E:518:ASN:HD22	1.39	0.87
1:E:112:ARG:HH12	1:E:190:GLN:NE2	1.72	0.86
1:C:588:HIS:HD2	1:C:590:LEU:H	1.20	0.86
1:B:13:CYS:O	1:B:17:GLU:HG3	1.76	0.86
1:A:533:GLN:H	1:A:533:GLN:HE21	0.90	0.85
1:D:533:GLN:HE21	1:D:533:GLN:N	1.73	0.85
1:F:258:SER:HA	1:F:302:SER:HA	1.55	0.85
1:A:515:LEU:HD22	1:A:525:ILE:HG23	1.60	0.84
1:D:588:HIS:CD2	1:D:590:LEU:H	1.95	0.83
1:E:601:ARG:HH11	1:E:601:ARG:CB	1.92	0.82
1:B:515:LEU:HD22	1:B:525:ILE:HG23	1.62	0.82
1:E:112:ARG:HH12	1:E:190:GLN:HE22	0.86	0.82
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.61	0.82
1:F:64:HIS:NE2	1:F:66:LEU:HD13	1.95	0.82
1:C:16:ILE:HD13	1:C:29:ILE:HD13	1.61	0.81
1:D:515:LEU:HA	1:D:518:ASN:HD22	1.46	0.81
1:B:601:ARG:CB	1:B:601:ARG:HH11	1.93	0.81
1:D:368:ASP:H	1:D:372:HIS:CD2	1.97	0.80
1:C:112:ARG:NH1	1:C:190:GLN:HE22	1.78	0.80
1:B:16:ILE:HD13	1:B:29:ILE:HD13	1.62	0.80
1:B:588:HIS:CD2	1:B:590:LEU:H	2.00	0.80
1:D:13:CYS:O	1:D:17:GLU:HG3	1.82	0.80
1:D:588:HIS:HD2	1:D:590:LEU:H	1.25	0.80
1:B:245:SER:HB2	1:B:274:LEU:HD11	1.63	0.79
1:A:258:SER:HA	1:A:302:SER:HA	1.64	0.79
1:F:207:PHE:CZ	1:F:304:LEU:HD11	2.18	0.79
1:E:1:MET:HE2	1:E:77:ASP:HB3	1.65	0.78
1:A:245:SER:HB2	1:A:274:LEU:HD11	1.65	0.78
1:E:588:HIS:CD2	1:E:590:LEU:H	2.01	0.78
1:E:13:CYS:O	1:E:17:GLU:HG3	1.83	0.78
1:F:16:ILE:HD13	1:F:29:ILE:HD13	1.64	0.77
1:F:588:HIS:CD2	1:F:590:LEU:H	2.02	0.77
1:F:107:LEU:HD21	1:F:149:ARG:HG2	1.66	0.77
1:C:515:LEU:HD22	1:C:525:ILE:HG23	1.67	0.77
1:B:234:TYR:CE1	1:B:239:LYS:HB2	2.21	0.76
1:F:515:LEU:HD22	1:F:525:ILE:HG23	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:ASP:OD2	1:A:227:PRO:HA	1.85	0.76
1:A:112:ARG:NH1	1:A:190:GLN:HE22	1.78	0.75
1:A:588:HIS:CD2	1:A:590:LEU:H	2.04	0.75
1:C:601:ARG:HH11	1:C:601:ARG:CB	2.00	0.75
1:C:13:CYS:O	1:C:17:GLU:HG3	1.84	0.75
1:F:588:HIS:HD2	1:F:590:LEU:H	1.36	0.74
1:B:324:ASN:HD22	1:B:353:ILE:HG13	1.53	0.74
1:D:112:ARG:NH1	1:D:190:GLN:HE22	1.82	0.74
1:A:434:GLU:CD	1:A:460:ARG:HH21	1.95	0.74
1:A:601:ARG:CB	1:A:601:ARG:HH11	2.01	0.74
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.68	0.74
1:A:460:ARG:HD3	1:A:614:GLN:O	1.87	0.73
1:F:112:ARG:NH1	1:F:190:GLN:HE22	1.82	0.73
1:C:173:LEU:O	1:C:177:LEU:HB2	1.88	0.73
1:B:258:SER:HA	1:B:302:SER:HA	1.71	0.73
1:D:460:ARG:HD3	1:D:614:GLN:O	1.87	0.73
1:D:636:ILE:HD12	1:D:636:ILE:H	1.54	0.73
1:E:258:SER:HA	1:E:302:SER:HA	1.71	0.73
1:A:16:ILE:HD13	1:A:29:ILE:HD13	1.70	0.72
1:E:655:LEU:O	1:E:656:THR:HG23	1.89	0.72
1:B:460:ARG:HD3	1:B:614:GLN:O	1.89	0.72
1:E:434:GLU:CD	1:E:460:ARG:HH21	1.97	0.72
1:B:173:LEU:O	1:B:177:LEU:HB2	1.89	0.72
1:D:1:MET:HE2	1:D:77:ASP:HB3	1.70	0.72
1:A:655:LEU:O	1:A:656:THR:HG23	1.90	0.72
1:A:213:PRO:HD2	1:A:216:VAL:HG21	1.71	0.72
1:C:3:THR:HG22	1:C:78:VAL:HG13	1.71	0.72
1:D:207:PHE:CZ	1:D:304:LEU:HD11	2.25	0.72
1:A:207:PHE:CZ	1:A:304:LEU:HD11	2.25	0.71
1:C:434:GLU:CD	1:C:460:ARG:HH21	1.98	0.71
1:D:3:THR:HG22	1:D:78:VAL:HG13	1.72	0.71
1:A:234:TYR:CE1	1:A:239:LYS:HB2	2.25	0.71
1:E:78:VAL:HB	1:E:98:ALA:HB3	1.71	0.71
1:F:14:LEU:HD12	1:F:15:GLY:N	2.05	0.71
1:D:63:ASN:HB3	1:D:89:TYR:CZ	2.25	0.71
1:F:636:ILE:HD12	1:F:636:ILE:H	1.55	0.71
1:F:601:ARG:CB	1:F:601:ARG:HH11	2.04	0.71
1:A:636:ILE:HD12	1:A:636:ILE:H	1.55	0.71
1:A:63:ASN:HB3	1:A:89:TYR:CZ	2.25	0.71
1:D:601:ARG:CB	1:D:601:ARG:HH11	2.04	0.71
1:D:107:LEU:HD21	1:D:149:ARG:HG2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:63:ASN:HB3	1:F:89:TYR:CZ	2.25	0.70
1:F:324:ASN:HD21	1:F:352:ALA:H	1.37	0.70
1:B:588:HIS:HD2	1:B:590:LEU:H	1.37	0.70
1:E:138:ARG:HH12	1:E:192:GLU:CD	1.99	0.70
1:C:1:MET:HE2	1:C:77:ASP:HB3	1.73	0.70
1:B:226:ASP:OD2	1:B:227:PRO:HA	1.92	0.70
1:C:460:ARG:HD3	1:C:614:GLN:O	1.91	0.70
1:D:226:ASP:OD2	1:D:227:PRO:HA	1.92	0.70
1:C:226:ASP:OD2	1:C:227:PRO:HA	1.92	0.70
1:C:324:ASN:HD22	1:C:353:ILE:HG13	1.56	0.70
1:B:11:MET:HG3	1:B:83:TYR:CE1	2.26	0.69
1:B:636:ILE:HD12	1:B:636:ILE:H	1.57	0.69
1:C:245:SER:HB2	1:C:274:LEU:HD11	1.73	0.69
1:C:517:LEU:O	1:C:521:GLU:HG2	1.91	0.69
1:A:515:LEU:HA	1:A:518:ASN:HD22	1.57	0.69
1:D:64:HIS:HD2	1:D:66:LEU:HB2	1.57	0.69
1:F:655:LEU:O	1:F:656:THR:HG23	1.92	0.69
1:B:63:ASN:HB3	1:B:89:TYR:CZ	2.28	0.69
1:E:16:ILE:HD13	1:E:29:ILE:HD13	1.72	0.69
1:F:19:LEU:HD11	1:F:80:PHE:CE2	2.28	0.69
1:B:112:ARG:HH12	1:B:190:GLN:HE22	0.82	0.69
1:C:636:ILE:HD12	1:C:636:ILE:H	1.58	0.69
1:F:434:GLU:CD	1:F:460:ARG:HH21	2.00	0.69
1:F:173:LEU:O	1:F:177:LEU:HB2	1.93	0.69
1:B:134:ARG:O	1:B:142:GLY:HA3	1.92	0.68
1:A:1:MET:N	1:A:181:LYS:HE3	2.07	0.68
1:A:244:SER:CB	1:A:277:VAL:HB	2.23	0.68
1:B:422:LYS:HD3	1:B:423:TYR:CE2	2.27	0.68
1:F:615:ASP:CG	1:F:616:VAL:H	2.00	0.68
1:D:138:ARG:HH12	1:D:192:GLU:CD	2.00	0.68
1:E:517:LEU:O	1:E:521:GLU:HG2	1.93	0.68
1:A:517:LEU:O	1:A:521:GLU:HG2	1.94	0.68
1:C:235:VAL:HG21	1:C:296:LEU:HD13	1.75	0.68
1:E:1:MET:HE1	1:E:98:ALA:HB2	1.75	0.68
1:E:226:ASP:OD2	1:E:227:PRO:HA	1.93	0.68
1:E:369:ILE:HD11	1:E:408:LEU:HD21	1.75	0.67
1:F:11:MET:HG3	1:F:83:TYR:CE1	2.28	0.67
1:B:3:THR:HG22	1:B:78:VAL:HG13	1.77	0.67
1:B:244:SER:CB	1:B:277:VAL:HB	2.25	0.67
1:C:112:ARG:HH12	1:C:190:GLN:NE2	1.81	0.67
1:C:526:LYS:HE3	1:C:603:VAL:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:LEU:O	1:E:177:LEU:HB2	1.93	0.67
1:C:3:THR:CG2	1:C:78:VAL:HG13	2.25	0.67
1:C:63:ASN:HB3	1:C:89:TYR:CZ	2.30	0.67
1:E:3:THR:HG22	1:E:78:VAL:HG13	1.77	0.67
1:E:11:MET:HG3	1:E:83:TYR:CE1	2.29	0.67
1:F:1:MET:HE1	1:F:98:ALA:CB	2.24	0.67
1:E:329:ASN:HD22	1:E:355:ARG:NH2	1.92	0.67
1:C:329:ASN:HD22	1:C:355:ARG:NH2	1.92	0.67
1:A:369:ILE:HD11	1:A:408:LEU:HD21	1.76	0.67
1:B:434:GLU:CD	1:B:460:ARG:HH21	2.02	0.67
1:E:368:ASP:H	1:E:372:HIS:CD2	2.05	0.67
1:F:422:LYS:HD3	1:F:423:TYR:CE2	2.30	0.67
1:F:3:THR:HG22	1:F:78:VAL:HG13	1.76	0.67
1:F:460:ARG:HD3	1:F:614:GLN:O	1.94	0.67
1:C:277:VAL:HG12	1:C:278:THR:HG23	1.78	0.66
1:D:11:MET:HG3	1:D:83:TYR:CE1	2.31	0.66
1:F:515:LEU:HA	1:F:518:ASN:HD22	1.60	0.66
1:C:368:ASP:H	1:C:372:HIS:CD2	2.05	0.66
1:E:107:LEU:HD21	1:E:149:ARG:HG2	1.77	0.66
1:F:138:ARG:HH12	1:F:192:GLU:CD	2.03	0.66
1:B:107:LEU:HD21	1:B:149:ARG:HG2	1.77	0.66
1:B:515:LEU:HA	1:B:518:ASN:ND2	2.08	0.66
1:C:655:LEU:O	1:C:656:THR:HG23	1.96	0.66
1:E:460:ARG:HD3	1:E:614:GLN:O	1.94	0.66
1:F:245:SER:HB2	1:F:274:LEU:HD11	1.77	0.66
1:D:16:ILE:HD13	1:D:29:ILE:HD13	1.76	0.66
1:A:422:LYS:HD3	1:A:423:TYR:CE2	2.31	0.66
1:C:615:ASP:CG	1:C:616:VAL:H	2.03	0.66
1:C:234:TYR:CE1	1:C:239:LYS:HB2	2.29	0.66
1:E:636:ILE:H	1:E:636:ILE:HD12	1.58	0.66
1:F:368:ASP:H	1:F:372:HIS:CD2	2.05	0.66
1:E:134:ARG:O	1:E:142:GLY:HA3	1.94	0.66
1:C:244:SER:CB	1:C:277:VAL:HB	2.26	0.66
1:D:329:ASN:HD22	1:D:355:ARG:NH2	1.94	0.66
1:D:434:GLU:CD	1:D:460:ARG:HH21	2.03	0.65
1:F:134:ARG:O	1:F:142:GLY:HA3	1.97	0.65
1:A:1:MET:HE2	1:A:77:ASP:HB3	1.77	0.65
1:E:324:ASN:HD21	1:E:352:ALA:H	1.42	0.65
1:F:329:ASN:HD22	1:F:355:ARG:NH2	1.95	0.65
1:D:649:PHE:O	1:D:652:THR:HB	1.96	0.65
1:A:324:ASN:HD21	1:A:352:ALA:H	1.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:369:ILE:HD11	1:B:408:LEU:HD21	1.77	0.65
1:C:211:HIS:O	1:C:270:GLY:HA3	1.97	0.65
1:D:258:SER:HA	1:D:302:SER:HA	1.77	0.65
1:A:11:MET:HG3	1:A:83:TYR:CE1	2.31	0.65
1:B:368:ASP:H	1:B:372:HIS:CD2	2.07	0.65
1:F:108:LEU:HD12	1:F:131:THR:HG21	1.79	0.65
1:F:211:HIS:O	1:F:270:GLY:HA3	1.97	0.65
1:F:213:PRO:HD2	1:F:216:VAL:HG21	1.77	0.65
1:B:1:MET:HE2	1:B:77:ASP:HB3	1.79	0.65
1:C:107:LEU:HD21	1:C:149:ARG:HG2	1.79	0.65
1:D:324:ASN:HD21	1:D:352:ALA:H	1.45	0.64
1:B:655:LEU:O	1:B:656:THR:HG23	1.96	0.64
1:E:64:HIS:HD2	1:E:66:LEU:HB2	1.61	0.64
1:A:588:HIS:HD2	1:A:590:LEU:H	1.44	0.64
1:A:615:ASP:CG	1:A:616:VAL:H	2.06	0.64
1:F:526:LYS:HE3	1:F:603:VAL:HG21	1.80	0.64
1:A:329:ASN:HD22	1:A:355:ARG:NH2	1.96	0.64
1:B:207:PHE:CZ	1:B:304:LEU:HD11	2.33	0.64
1:B:64:HIS:HD2	1:B:66:LEU:HB2	1.63	0.64
1:B:517:LEU:O	1:B:521:GLU:HG2	1.98	0.64
1:F:422:LYS:HD3	1:F:423:TYR:CZ	2.33	0.64
1:B:347:ASP:OD1	1:B:348:ILE:N	2.31	0.64
1:E:567:ASN:ND2	1:E:569:GLU:H	1.94	0.64
1:F:64:HIS:HD2	1:F:66:LEU:HB2	1.61	0.64
1:B:403:LEU:O	1:B:407:GLU:HG3	1.98	0.64
1:C:431:SER:HB3	1:C:489:ARG:HG2	1.79	0.64
1:E:541:ARG:NH1	1:E:636:ILE:HG12	2.13	0.64
1:C:515:LEU:HA	1:C:518:ASN:ND2	2.13	0.64
1:C:649:PHE:O	1:C:652:THR:HB	1.98	0.64
1:D:3:THR:CG2	1:D:78:VAL:HG13	2.29	0.63
1:D:541:ARG:NH1	1:D:636:ILE:HG12	2.13	0.63
1:A:597:PHE:CE2	1:A:599:GLY:HA2	2.33	0.63
1:B:615:ASP:CG	1:B:616:VAL:H	2.06	0.63
1:E:422:LYS:HD3	1:E:423:TYR:CE2	2.33	0.63
1:D:1:MET:HE1	1:D:98:ALA:HB2	1.81	0.63
1:E:588:HIS:HD2	1:E:590:LEU:H	1.44	0.63
1:A:324:ASN:HD22	1:A:353:ILE:HG13	1.62	0.63
1:D:403:LEU:O	1:D:407:GLU:HG3	1.98	0.63
1:F:235:VAL:HG21	1:F:296:LEU:HD13	1.81	0.63
1:D:1:MET:N	1:D:181:LYS:HE3	2.14	0.63
1:C:6:PHE:HZ	1:C:92:ILE:HD11	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ARG:O	1:C:142:GLY:HA3	1.99	0.63
1:E:63:ASN:HB3	1:E:89:TYR:CZ	2.34	0.63
1:A:173:LEU:O	1:A:177:LEU:HB2	1.99	0.62
1:D:573:SER:OG	1:D:576:GLU:HG3	1.99	0.62
1:A:107:LEU:HD21	1:A:149:ARG:HG2	1.80	0.62
1:F:324:ASN:HD21	1:F:352:ALA:N	1.96	0.62
1:D:134:ARG:O	1:D:142:GLY:HA3	1.98	0.62
1:F:346:LEU:C	1:F:346:LEU:HD23	2.25	0.62
1:A:89:TYR:C	1:A:93:LEU:HD23	2.25	0.62
1:D:593:HIS:CG	1:D:655:LEU:HD13	2.34	0.62
1:D:615:ASP:CG	1:D:616:VAL:H	2.06	0.62
1:F:244:SER:CB	1:F:277:VAL:HB	2.29	0.62
1:F:277:VAL:HG12	1:F:278:THR:HG23	1.80	0.62
1:D:14:LEU:HD12	1:D:15:GLY:N	2.14	0.62
1:D:369:ILE:HD12	1:D:412:GLU:HB3	1.82	0.62
1:F:226:ASP:OD2	1:F:227:PRO:HA	2.00	0.62
1:A:277:VAL:HG12	1:A:278:THR:HG23	1.81	0.62
1:A:524:PRO:HD3	1:C:297:GLY:HA3	1.80	0.62
1:A:526:LYS:HE3	1:A:603:VAL:HG21	1.81	0.62
1:D:368:ASP:N	1:D:372:HIS:HD2	1.88	0.62
1:E:573:SER:OG	1:E:576:GLU:HG3	2.00	0.62
1:B:138:ARG:HH12	1:B:192:GLU:CD	2.06	0.62
1:D:588:HIS:HE1	1:D:647:ASP:OD1	1.83	0.62
1:E:588:HIS:HE1	1:E:647:ASP:OD1	1.83	0.62
1:A:213:PRO:HD2	1:A:216:VAL:CG2	2.29	0.61
1:B:338:GLU:HG3	1:B:548:TYR:OH	2.00	0.61
1:C:11:MET:HG3	1:C:83:TYR:CE1	2.34	0.61
1:C:573:SER:OG	1:C:576:GLU:HG3	1.99	0.61
1:F:369:ILE:HD11	1:F:408:LEU:HD21	1.82	0.61
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.65	0.61
1:D:517:LEU:O	1:D:521:GLU:HG2	2.00	0.61
1:E:234:TYR:CE1	1:E:239:LYS:HB2	2.35	0.61
1:E:567:ASN:C	1:E:567:ASN:HD22	2.07	0.61
1:C:368:ASP:N	1:C:372:HIS:HD2	1.94	0.61
1:C:369:ILE:HD11	1:C:408:LEU:HD21	1.82	0.61
1:A:3:THR:HG22	1:A:78:VAL:HG13	1.82	0.61
1:A:244:SER:HB3	1:A:277:VAL:HB	1.83	0.61
1:C:207:PHE:CZ	1:C:304:LEU:HD11	2.34	0.61
1:E:245:SER:HB2	1:E:274:LEU:HD11	1.82	0.61
1:E:567:ASN:HD21	1:E:569:GLU:HB2	1.65	0.61
1:B:422:LYS:HD3	1:B:423:TYR:CZ	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:HIS:HD2	1:C:66:LEU:HB2	1.65	0.61
1:D:64:HIS:CD2	1:D:66:LEU:HB2	2.36	0.61
1:E:150:ILE:HD12	1:E:165:LEU:HD23	1.82	0.61
1:F:573:SER:OG	1:F:576:GLU:HG3	2.00	0.61
1:A:346:LEU:C	1:A:346:LEU:HD23	2.26	0.61
1:B:501:LEU:H	1:B:501:LEU:HD22	1.64	0.61
1:C:138:ARG:HH12	1:C:192:GLU:CD	2.08	0.61
1:B:244:SER:HB2	1:B:277:VAL:HB	1.81	0.61
1:B:573:SER:OG	1:B:576:GLU:HG3	2.00	0.61
1:B:431:SER:HB3	1:B:489:ARG:HG2	1.83	0.61
1:E:277:VAL:HG12	1:E:278:THR:HG23	1.83	0.61
1:F:244:SER:HB3	1:F:277:VAL:HB	1.82	0.61
1:A:460:ARG:O	1:A:460:ARG:HG3	1.98	0.60
1:C:588:HIS:HE1	1:C:647:ASP:OD1	1.84	0.60
1:D:78:VAL:HB	1:D:98:ALA:HB3	1.83	0.60
1:A:64:HIS:HD2	1:A:66:LEU:HB2	1.65	0.60
1:C:469:LEU:HD12	1:F:469:LEU:HD12	1.82	0.60
1:D:567:ASN:HD21	1:D:569:GLU:HB2	1.66	0.60
1:E:615:ASP:CG	1:E:616:VAL:H	2.09	0.60
1:F:575:GLU:O	1:F:579:GLU:HG3	2.00	0.60
1:D:424:ARG:HG2	1:D:424:ARG:HH11	1.66	0.60
1:B:575:GLU:O	1:B:579:GLU:HG3	2.01	0.60
1:E:422:LYS:HD3	1:E:423:TYR:CZ	2.36	0.60
1:A:134:ARG:O	1:A:142:GLY:HA3	2.00	0.60
1:C:6:PHE:CZ	1:C:92:ILE:HD11	2.36	0.60
1:C:113:GLY:HA3	1:C:198:PHE:H	1.67	0.60
1:E:64:HIS:NE2	1:E:66:LEU:HD13	2.16	0.60
1:F:234:TYR:CE1	1:F:239:LYS:HB2	2.37	0.60
1:F:517:LEU:O	1:F:521:GLU:HG2	2.01	0.60
1:D:515:LEU:HA	1:D:518:ASN:ND2	2.17	0.60
1:E:207:PHE:CZ	1:E:304:LEU:HD11	2.36	0.60
1:F:1:MET:HE2	1:F:77:ASP:CB	2.28	0.60
1:B:424:ARG:HG2	1:B:424:ARG:HH11	1.66	0.60
1:A:138:ARG:HH12	1:A:192:GLU:CD	2.09	0.60
1:E:252:SER:C	1:E:254:ALA:H	2.10	0.60
1:C:593:HIS:CG	1:C:655:LEU:HD13	2.37	0.59
1:D:434:GLU:HG2	1:D:464:SER:HB2	1.84	0.59
1:F:99:GLY:HA3	1:F:134:ARG:HH12	1.67	0.59
1:A:369:ILE:HD11	1:A:408:LEU:CD2	2.33	0.59
1:F:107:LEU:HD13	1:F:129:GLY:HA3	1.84	0.59
1:B:329:ASN:HD22	1:B:355:ARG:NH2	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:567:ASN:ND2	1:F:569:GLU:H	2.00	0.59
1:D:460:ARG:O	1:D:460:ARG:HG3	1.98	0.59
1:E:102:ASN:HD22	1:E:133:HIS:CE1	2.21	0.59
1:A:64:HIS:NE2	1:A:66:LEU:HD13	2.17	0.59
1:A:244:SER:HB2	1:A:277:VAL:HB	1.85	0.59
1:D:245:SER:HB2	1:D:274:LEU:HD11	1.83	0.59
1:B:64:HIS:NE2	1:B:66:LEU:HD13	2.18	0.59
1:C:244:SER:HB2	1:C:277:VAL:HB	1.84	0.59
1:C:588:HIS:HD2	1:C:590:LEU:N	1.97	0.59
1:D:347:ASP:OD1	1:D:348:ILE:N	2.36	0.59
1:E:324:ASN:HD21	1:E:352:ALA:N	2.00	0.59
1:F:541:ARG:NH1	1:F:636:ILE:HG12	2.17	0.59
1:F:108:LEU:HD12	1:F:131:THR:CG2	2.32	0.59
1:B:369:ILE:HD11	1:B:408:LEU:CD2	2.33	0.59
1:C:107:LEU:HD13	1:C:129:GLY:HA3	1.83	0.59
1:C:403:LEU:O	1:C:407:GLU:HG3	2.03	0.59
1:A:431:SER:HB3	1:A:489:ARG:HG2	1.85	0.58
1:B:601:ARG:HH11	1:B:601:ARG:HB2	1.68	0.58
1:C:434:GLU:HG2	1:C:464:SER:HB2	1.85	0.58
1:C:597:PHE:CE2	1:C:599:GLY:HA2	2.38	0.58
1:D:526:LYS:HE3	1:D:603:VAL:HG21	1.85	0.58
1:F:1:MET:N	1:F:181:LYS:HE3	2.18	0.58
1:A:422:LYS:HD3	1:A:423:TYR:CZ	2.37	0.58
1:C:347:ASP:OD1	1:C:348:ILE:N	2.37	0.58
1:F:6:PHE:HZ	1:F:92:ILE:HD11	1.68	0.58
1:F:109:PRO:HB2	1:F:195:ALA:HB2	1.85	0.58
1:A:172:LEU:C	1:A:172:LEU:HD23	2.29	0.58
1:B:252:SER:C	1:B:254:ALA:H	2.10	0.58
1:B:369:ILE:HD12	1:B:412:GLU:HB3	1.84	0.58
1:E:649:PHE:O	1:E:652:THR:HB	2.03	0.58
1:F:70:ARG:O	1:F:73:GLN:HB2	2.03	0.58
1:F:324:ASN:HD22	1:F:353:ILE:HG13	1.69	0.58
1:A:70:ARG:O	1:A:73:GLN:HB2	2.04	0.58
1:A:588:HIS:HE1	1:A:647:ASP:OD1	1.85	0.58
1:B:346:LEU:C	1:B:346:LEU:HD23	2.28	0.58
1:B:368:ASP:N	1:B:372:HIS:HD2	1.95	0.58
1:C:89:TYR:C	1:C:93:LEU:HD23	2.28	0.58
1:C:369:ILE:CD1	1:C:390:VAL:HG11	2.34	0.58
1:C:541:ARG:NH1	1:C:636:ILE:HG12	2.19	0.58
1:D:113:GLY:HA3	1:D:198:PHE:H	1.69	0.58
1:D:234:TYR:CE1	1:D:239:LYS:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:LEU:C	1:D:346:LEU:HD23	2.28	0.58
1:E:369:ILE:HD11	1:E:408:LEU:CD2	2.33	0.58
1:E:515:LEU:HA	1:E:518:ASN:ND2	2.15	0.58
1:A:78:VAL:HB	1:A:98:ALA:HB3	1.83	0.58
1:A:501:LEU:HD22	1:A:501:LEU:H	1.69	0.58
1:A:368:ASP:H	1:A:372:HIS:CD2	2.09	0.58
1:B:113:GLY:HA3	1:B:198:PHE:H	1.67	0.58
1:D:324:ASN:HD22	1:D:353:ILE:HG13	1.69	0.58
1:D:499:ASP:HB2	1:D:513:THR:HG21	1.85	0.58
1:F:567:ASN:C	1:F:567:ASN:HD22	2.12	0.58
1:A:541:ARG:NH1	1:A:636:ILE:HG12	2.18	0.57
1:B:3:THR:HG22	1:B:78:VAL:CG1	2.33	0.57
1:D:64:HIS:NE2	1:D:66:LEU:HD13	2.18	0.57
1:D:172:LEU:C	1:D:172:LEU:HD23	2.29	0.57
1:E:6:PHE:CZ	1:E:92:ILE:HD11	2.39	0.57
1:E:244:SER:HB2	1:E:277:VAL:HB	1.85	0.57
1:A:369:ILE:HD12	1:A:412:GLU:HB3	1.84	0.57
1:E:1:MET:N	1:E:181:LYS:HE3	2.19	0.57
1:D:1:MET:HE1	1:D:98:ALA:CB	2.35	0.57
1:F:499:ASP:HB2	1:F:513:THR:HG21	1.86	0.57
1:D:99:GLY:HA3	1:D:134:ARG:HH12	1.69	0.57
1:E:346:LEU:C	1:E:346:LEU:HD23	2.29	0.57
1:A:465:VAL:HG21	1:D:468:GLN:OE1	2.04	0.57
1:E:14:LEU:C	1:E:14:LEU:HD12	2.29	0.57
1:E:64:HIS:CD2	1:E:66:LEU:HB2	2.40	0.57
1:F:567:ASN:HD21	1:F:569:GLU:HB2	1.69	0.57
1:F:588:HIS:HE1	1:F:647:ASP:OD1	1.88	0.57
1:A:649:PHE:O	1:A:652:THR:HB	2.05	0.57
1:B:526:LYS:HE3	1:B:603:VAL:HG21	1.86	0.57
1:C:64:HIS:NE2	1:C:66:LEU:HD13	2.20	0.57
1:C:575:GLU:O	1:C:579:GLU:HG3	2.04	0.57
1:D:213:PRO:HD2	1:D:216:VAL:HG21	1.86	0.57
1:D:655:LEU:O	1:D:656:THR:HG23	2.04	0.57
1:F:375:TRP:O	1:F:379:HIS:HD2	1.88	0.57
1:E:347:ASP:OD1	1:E:348:ILE:N	2.37	0.57
1:D:324:ASN:HD21	1:D:352:ALA:N	2.02	0.57
1:D:567:ASN:C	1:D:567:ASN:HD22	2.11	0.57
1:E:6:PHE:HZ	1:E:92:ILE:HD11	1.70	0.57
1:E:434:GLU:HG2	1:E:464:SER:HB2	1.86	0.57
1:B:172:LEU:C	1:B:172:LEU:HD23	2.29	0.57
1:C:324:ASN:HD21	1:C:352:ALA:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:ASN:ND2	1:D:569:GLU:H	2.02	0.57
1:E:368:ASP:N	1:E:372:HIS:HD2	1.93	0.57
1:F:89:TYR:C	1:F:93:LEU:HD23	2.30	0.57
1:A:107:LEU:HD13	1:A:129:GLY:HA3	1.86	0.57
1:B:235:VAL:HG21	1:B:296:LEU:HD13	1.87	0.57
1:F:369:ILE:HD12	1:F:412:GLU:HB3	1.87	0.57
1:A:299:VAL:O	1:A:301:GLY:N	2.38	0.56
1:E:369:ILE:CD1	1:E:390:VAL:HG11	2.35	0.56
1:E:424:ARG:HG2	1:E:424:ARG:HH11	1.68	0.56
1:B:67:TRP:NE1	1:E:604:GLU:OE2	2.30	0.56
1:C:70:ARG:O	1:C:73:GLN:HB2	2.05	0.56
1:C:338:GLU:HG3	1:C:548:TYR:OH	2.05	0.56
1:E:324:ASN:HD22	1:E:353:ILE:HG13	1.69	0.56
1:E:235:VAL:HG21	1:E:296:LEU:HD13	1.86	0.56
1:B:649:PHE:O	1:B:652:THR:HB	2.05	0.56
1:C:567:ASN:C	1:C:567:ASN:HD22	2.11	0.56
1:D:369:ILE:HD11	1:D:408:LEU:HD21	1.87	0.56
1:E:244:SER:CB	1:E:277:VAL:HB	2.34	0.56
1:E:601:ARG:HH11	1:E:601:ARG:HB2	1.68	0.56
1:F:3:THR:CG2	1:F:78:VAL:HG13	2.35	0.56
1:F:146:ALA:CB	1:F:176:THR:HG21	2.36	0.56
1:F:460:ARG:O	1:F:460:ARG:HG3	2.01	0.56
1:E:1:MET:HE1	1:E:98:ALA:CB	2.36	0.56
1:B:121:LEU:O	1:B:219:ASN:HB3	2.05	0.56
1:F:347:ASP:OD1	1:F:348:ILE:N	2.38	0.56
1:C:213:PRO:HD2	1:C:216:VAL:HG21	1.88	0.56
1:B:499:ASP:HB2	1:B:513:THR:HG21	1.88	0.56
1:C:90:ASP:O	1:C:91:GLU:C	2.48	0.56
1:A:515:LEU:HA	1:A:518:ASN:ND2	2.21	0.55
1:C:422:LYS:HD3	1:C:423:TYR:CZ	2.41	0.55
1:C:422:LYS:HD3	1:C:423:TYR:CE2	2.42	0.55
1:D:92:ILE:O	1:D:95:LEU:HG	2.06	0.55
1:E:150:ILE:CD1	1:E:165:LEU:HD23	2.36	0.55
1:E:567:ASN:HD22	1:E:569:GLU:H	1.54	0.55
1:C:92:ILE:O	1:C:95:LEU:HG	2.06	0.55
1:E:172:LEU:C	1:E:172:LEU:HD23	2.31	0.55
1:C:1:MET:N	1:C:181:LYS:HE3	2.21	0.55
1:B:246:ARG:HB3	1:B:275:GLU:HB3	1.87	0.55
1:C:346:LEU:HD23	1:C:346:LEU:C	2.32	0.55
1:D:89:TYR:C	1:D:93:LEU:HD23	2.31	0.55
1:F:90:ASP:O	1:F:94:GLN:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:424:ARG:HG2	1:F:424:ARG:HH11	1.71	0.55
1:A:347:ASP:OD1	1:A:348:ILE:N	2.39	0.55
1:B:244:SER:HB3	1:B:277:VAL:HB	1.89	0.55
1:C:465:VAL:HG21	1:F:468:GLN:OE1	2.06	0.55
1:D:3:THR:HG22	1:D:78:VAL:CG1	2.36	0.55
1:B:324:ASN:HD21	1:B:352:ALA:H	1.54	0.55
1:C:567:ASN:HD21	1:C:569:GLU:HB2	1.72	0.55
1:D:235:VAL:HG21	1:D:296:LEU:HD13	1.89	0.55
1:E:601:ARG:HH11	1:E:601:ARG:HB3	1.68	0.55
1:F:368:ASP:N	1:F:372:HIS:HD2	1.94	0.55
1:A:92:ILE:O	1:A:95:LEU:HG	2.07	0.55
1:D:431:SER:HB3	1:D:489:ARG:HG2	1.88	0.55
1:A:325:GLY:HA3	2:A:1001:ATP:H5'2	1.89	0.55
1:A:573:SER:OG	1:A:576:GLU:HG3	2.07	0.55
1:C:115:ALA:N	1:C:116:PRO:CD	2.70	0.55
1:C:615:ASP:CG	1:C:616:VAL:N	2.65	0.55
1:F:501:LEU:HD22	1:F:501:LEU:H	1.71	0.55
1:C:499:ASP:HB2	1:C:513:THR:HG21	1.88	0.55
1:E:14:LEU:HD12	1:E:15:GLY:N	2.22	0.55
1:E:460:ARG:O	1:E:460:ARG:HG3	2.01	0.55
1:F:6:PHE:CZ	1:F:92:ILE:HD11	2.42	0.55
1:A:114:ARG:O	1:A:115:ALA:HB3	2.07	0.55
1:A:150:ILE:HD12	1:A:165:LEU:HD23	1.88	0.55
1:A:150:ILE:CD1	1:A:165:LEU:HD23	2.37	0.55
1:A:600:PHE:O	1:A:601:ARG:HG3	2.07	0.55
1:D:277:VAL:HG12	1:D:278:THR:HG23	1.88	0.55
1:D:369:ILE:HD11	1:D:408:LEU:CD2	2.37	0.55
1:E:545:GLU:O	1:E:549:ARG:HG2	2.07	0.55
1:A:109:PRO:O	1:A:195:ALA:HA	2.07	0.54
1:B:324:ASN:HD21	1:B:352:ALA:N	2.05	0.54
1:E:436:TYR:HA	1:E:451:LEU:HD22	1.89	0.54
1:F:71:ILE:HD12	1:F:92:ILE:HD12	1.89	0.54
1:F:434:GLU:HG2	1:F:464:SER:HB2	1.89	0.54
1:A:567:ASN:C	1:A:567:ASN:HD22	2.15	0.54
1:B:567:ASN:ND2	1:B:569:GLU:H	2.05	0.54
1:A:601:ARG:NH2	1:C:294:GLN:O	2.37	0.54
1:B:3:THR:CG2	1:B:78:VAL:HG13	2.36	0.54
1:B:369:ILE:CD1	1:B:390:VAL:HG11	2.37	0.54
1:C:324:ASN:HD21	1:C:352:ALA:N	2.06	0.54
1:D:422:LYS:HD3	1:D:423:TYR:CE2	2.42	0.54
1:B:469:LEU:HD12	1:E:469:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:GLU:O	1:D:73:GLN:HG2	2.08	0.54
1:D:115:ALA:N	1:D:116:PRO:CD	2.69	0.54
1:D:173:LEU:O	1:D:177:LEU:HB2	2.08	0.54
1:E:3:THR:CG2	1:E:78:VAL:HG13	2.37	0.54
1:F:1:MET:HE1	1:F:98:ALA:HB2	1.89	0.54
1:F:403:LEU:O	1:F:407:GLU:HG3	2.07	0.54
1:C:489:ARG:HB2	1:C:564:ASN:HD22	1.72	0.54
1:A:399:THR:HG22	1:A:459:PRO:HG2	1.89	0.54
1:B:201:ARG:NH2	1:B:220:MET:HE1	2.23	0.54
1:B:541:ARG:NH1	1:B:636:ILE:HG12	2.23	0.54
1:F:112:ARG:HH12	1:F:190:GLN:NE2	1.86	0.54
1:A:78:VAL:HG23	1:A:99:GLY:O	2.07	0.54
1:A:252:SER:C	1:A:254:ALA:H	2.16	0.54
1:E:89:TYR:C	1:E:93:LEU:HD23	2.33	0.54
1:E:211:HIS:O	1:E:270:GLY:HA3	2.08	0.54
1:B:324:ASN:ND2	1:B:353:ILE:HG13	2.20	0.54
1:C:244:SER:HB3	1:C:277:VAL:HB	1.89	0.54
1:F:180:ILE:HG12	1:F:185:ILE:HG21	1.90	0.54
1:B:434:GLU:HG2	1:B:464:SER:HB2	1.89	0.54
1:C:369:ILE:HD12	1:C:412:GLU:HB3	1.90	0.54
1:D:14:LEU:HD12	1:D:14:LEU:C	2.33	0.54
1:F:9:HIS:CG	1:F:10:ASP:H	2.26	0.54
1:F:64:HIS:CD2	1:F:66:LEU:HB2	2.41	0.54
1:F:615:ASP:CG	1:F:616:VAL:N	2.65	0.54
1:F:649:PHE:O	1:F:652:THR:HB	2.08	0.54
1:A:113:GLY:HA3	1:A:198:PHE:H	1.72	0.54
1:A:113:GLY:HA3	1:A:198:PHE:O	2.06	0.54
1:C:78:VAL:HB	1:C:98:ALA:HB3	1.89	0.54
1:C:99:GLY:HA3	1:C:134:ARG:HH12	1.73	0.54
1:E:115:ALA:N	1:E:116:PRO:CD	2.70	0.54
1:E:499:ASP:HB2	1:E:513:THR:HG21	1.89	0.54
1:F:489:ARG:HB2	1:F:564:ASN:HD22	1.73	0.54
1:C:14:LEU:HD12	1:C:15:GLY:N	2.23	0.53
1:E:454:GLY:H	1:E:461:TRP:CD1	2.25	0.53
1:F:597:PHE:CE2	1:F:599:GLY:HA2	2.43	0.53
1:A:211:HIS:O	1:A:270:GLY:HA3	2.08	0.53
1:B:89:TYR:C	1:B:93:LEU:HD23	2.33	0.53
1:B:201:ARG:HH22	1:B:220:MET:HE1	1.72	0.53
1:B:601:ARG:HH11	1:B:601:ARG:HB3	1.71	0.53
1:B:567:ASN:HD22	1:B:567:ASN:C	2.14	0.53
1:B:600:PHE:O	1:B:601:ARG:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:ARG:HH11	1:C:424:ARG:HG2	1.73	0.53
1:E:213:PRO:HD2	1:E:216:VAL:HG21	1.91	0.53
1:F:213:PRO:HD2	1:F:216:VAL:CG2	2.38	0.53
1:F:252:SER:C	1:F:254:ALA:H	2.16	0.53
1:A:3:THR:CG2	1:A:78:VAL:HG13	2.38	0.53
1:A:338:GLU:HG3	1:A:548:TYR:OH	2.09	0.53
1:A:601:ARG:HH21	1:C:294:GLN:C	2.17	0.53
1:C:3:THR:HG22	1:C:78:VAL:CG1	2.38	0.53
1:D:79:ILE:HG13	1:D:96:ALA:HB2	1.89	0.53
1:F:369:ILE:HD11	1:F:408:LEU:CD2	2.38	0.53
1:F:545:GLU:O	1:F:549:ARG:HG2	2.08	0.53
1:A:9:HIS:CG	1:A:10:ASP:H	2.27	0.53
1:A:324:ASN:HD21	1:A:352:ALA:N	2.06	0.53
1:D:567:ASN:ND2	1:D:569:GLU:HB2	2.23	0.53
1:F:117:LEU:HD13	1:F:165:LEU:HD12	1.89	0.53
1:F:426:ARG:HG3	1:F:484:GLN:HG2	1.89	0.53
1:F:636:ILE:HD12	1:F:636:ILE:N	2.21	0.53
1:F:150:ILE:HD12	1:F:165:LEU:HD23	1.90	0.53
1:A:368:ASP:N	1:A:372:HIS:HD2	1.97	0.53
1:A:575:GLU:O	1:A:579:GLU:HG3	2.09	0.53
1:E:252:SER:C	1:E:254:ALA:N	2.67	0.53
1:B:92:ILE:O	1:B:95:LEU:HG	2.09	0.53
1:B:109:PRO:HB2	1:B:195:ALA:HB2	1.91	0.53
1:D:244:SER:CB	1:D:277:VAL:HB	2.39	0.53
1:F:159:ILE:HG23	1:F:160:THR:N	2.24	0.53
1:F:338:GLU:HG3	1:F:548:TYR:OH	2.09	0.53
1:A:201:ARG:HH22	1:A:220:MET:HE1	1.74	0.53
1:B:588:HIS:HD2	1:B:590:LEU:N	2.06	0.53
1:E:19:LEU:HD11	1:E:80:PHE:CE2	2.44	0.53
1:F:112:ARG:CB	1:F:112:ARG:HH11	2.21	0.53
1:C:600:PHE:O	1:C:601:ARG:HG3	2.09	0.52
1:D:454:GLY:H	1:D:461:TRP:CD1	2.27	0.52
1:A:295:THR:HA	1:B:601:ARG:NH2	2.24	0.52
1:E:78:VAL:HA	1:E:96:ALA:HB1	1.90	0.52
1:E:107:LEU:HD13	1:E:129:GLY:HA3	1.91	0.52
1:A:499:ASP:HB2	1:A:513:THR:HG21	1.91	0.52
1:B:576:GLU:O	1:B:580:MET:HG3	2.10	0.52
1:D:567:ASN:HD22	1:D:569:GLU:H	1.57	0.52
1:B:498:LEU:O	1:B:499:ASP:HB2	2.10	0.52
1:B:588:HIS:HE1	1:B:647:ASP:OD1	1.93	0.52
1:D:588:HIS:HD2	1:D:590:LEU:N	2.02	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:597:PHE:CE2	1:D:599:GLY:HA2	2.45	0.52
1:E:369:ILE:HD12	1:E:412:GLU:HB3	1.90	0.52
1:F:11:MET:HG3	1:F:83:TYR:CZ	2.44	0.52
1:F:246:ARG:HB3	1:F:275:GLU:HB3	1.90	0.52
1:F:506:ILE:HG23	1:F:506:ILE:O	2.08	0.52
1:A:102:ASN:HD22	1:A:133:HIS:CE1	2.28	0.52
1:A:235:VAL:HG21	1:A:296:LEU:HD13	1.90	0.52
1:B:121:LEU:HD21	1:B:161:LEU:HD22	1.91	0.52
1:C:567:ASN:ND2	1:C:569:GLU:H	2.07	0.52
1:C:636:ILE:HD12	1:C:636:ILE:N	2.23	0.52
1:A:1:MET:HE1	1:A:98:ALA:CB	2.39	0.52
1:A:452:ILE:HG12	1:D:452:ILE:HG12	1.91	0.52
1:B:252:SER:C	1:B:254:ALA:N	2.67	0.52
1:D:114:ARG:O	1:D:115:ALA:HB3	2.09	0.52
1:D:244:SER:HB2	1:D:277:VAL:HB	1.91	0.52
1:D:575:GLU:O	1:D:579:GLU:HG3	2.10	0.52
1:A:201:ARG:NH2	1:A:220:MET:HE1	2.25	0.52
1:B:1:MET:HE1	1:B:98:ALA:CB	2.39	0.52
1:B:460:ARG:O	1:B:460:ARG:HG3	2.08	0.52
1:B:528:ILE:HD13	3:B:1102:UGA:C2	2.39	0.52
1:C:14:LEU:HD12	1:C:14:LEU:C	2.35	0.52
1:C:64:HIS:CD2	1:C:66:LEU:H	2.28	0.52
1:B:69:GLU:O	1:B:73:GLN:HG2	2.09	0.52
1:B:78:VAL:HB	1:B:98:ALA:HB3	1.91	0.52
1:C:16:ILE:CD1	1:C:29:ILE:HD13	2.37	0.52
1:A:11:MET:HG3	1:A:83:TYR:CZ	2.45	0.52
1:E:119:TRP:CZ2	1:E:201:ARG:HG2	2.45	0.52
1:E:399:THR:HG22	1:E:459:PRO:HG2	1.92	0.52
1:F:348:ILE:HG12	2:F:1006:ATP:C2	2.44	0.52
1:A:206:SER:HA	1:A:220:MET:HE2	1.91	0.51
1:E:567:ASN:ND2	1:E:569:GLU:HB2	2.24	0.51
1:F:454:GLY:H	1:F:461:TRP:CD1	2.28	0.51
1:B:78:VAL:HA	1:B:96:ALA:HB1	1.90	0.51
1:B:159:ILE:HB	1:B:227:PRO:HD2	1.91	0.51
1:E:102:ASN:HD22	1:E:133:HIS:HE1	1.56	0.51
1:F:431:SER:HB3	1:F:489:ARG:HG2	1.93	0.51
1:F:576:GLU:O	1:F:580:MET:HG3	2.11	0.51
1:C:369:ILE:HD11	1:C:408:LEU:CD2	2.40	0.51
1:D:78:VAL:HG23	1:D:99:GLY:O	2.10	0.51
1:D:107:LEU:HD13	1:D:129:GLY:HA3	1.93	0.51
1:F:201:ARG:NH2	1:F:220:MET:HE1	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:19:LEU:HD11	1:D:80:PHE:CE2	2.45	0.51
1:D:498:LEU:O	1:D:499:ASP:HB2	2.10	0.51
1:D:506:ILE:HG23	1:D:506:ILE:O	2.09	0.51
1:E:108:LEU:HD12	1:E:131:THR:HG21	1.90	0.51
1:E:214:ALA:HB1	1:E:247:VAL:HG12	1.92	0.51
1:A:6:PHE:HZ	1:A:92:ILE:HD11	1.76	0.51
1:B:99:GLY:HA3	1:B:134:ARG:HH12	1.75	0.51
1:B:615:ASP:CG	1:B:616:VAL:N	2.69	0.51
1:C:498:LEU:O	1:C:499:ASP:HB2	2.09	0.51
1:A:246:ARG:HB3	1:A:275:GLU:HB3	1.93	0.51
1:A:434:GLU:HG2	1:A:464:SER:HB2	1.93	0.51
1:A:506:ILE:HG23	1:A:506:ILE:O	2.10	0.51
1:A:615:ASP:CG	1:A:616:VAL:N	2.67	0.51
1:C:172:LEU:HD23	1:C:172:LEU:C	2.36	0.51
1:A:454:GLY:H	1:A:461:TRP:CD1	2.29	0.51
1:A:604:GLU:OE2	1:D:67:TRP:NE1	2.40	0.51
1:B:14:LEU:HD12	1:B:14:LEU:C	2.36	0.51
1:B:567:ASN:HD21	1:B:569:GLU:HB2	1.76	0.51
1:C:102:ASN:HD22	1:C:133:HIS:CE1	2.28	0.51
1:C:468:GLN:OE1	1:F:465:VAL:HG21	2.10	0.51
1:B:14:LEU:HD12	1:B:15:GLY:N	2.25	0.51
1:B:107:LEU:HD13	1:B:129:GLY:HA3	1.92	0.51
1:B:115:ALA:N	1:B:116:PRO:CD	2.74	0.51
1:B:597:PHE:CE2	1:B:599:GLY:HA2	2.46	0.51
1:C:342:GLU:OE2	1:C:363:HIS:HE1	1.94	0.51
1:B:452:ILE:HG12	1:E:452:ILE:HG12	1.92	0.51
1:C:64:HIS:CD2	1:C:66:LEU:HB2	2.46	0.51
1:E:597:PHE:CE2	1:E:599:GLY:HA2	2.46	0.51
1:F:113:GLY:HA3	1:F:198:PHE:H	1.76	0.51
1:E:99:GLY:HA3	1:E:134:ARG:HH12	1.76	0.50
1:A:117:LEU:HD13	1:A:165:LEU:HD12	1.93	0.50
1:A:567:ASN:ND2	1:A:569:GLU:H	2.10	0.50
1:B:146:ALA:CB	1:B:176:THR:HG21	2.42	0.50
1:C:369:ILE:HD11	1:C:390:VAL:HG11	1.92	0.50
1:D:636:ILE:HD12	1:D:636:ILE:N	2.24	0.50
1:E:575:GLU:O	1:E:579:GLU:HG3	2.10	0.50
1:A:115:ALA:N	1:A:116:PRO:CD	2.74	0.50
1:D:90:ASP:O	1:D:94:GLN:HG2	2.11	0.50
1:E:338:GLU:HG3	1:E:548:TYR:OH	2.11	0.50
1:B:70:ARG:O	1:B:73:GLN:HB2	2.11	0.50
1:C:324:ASN:ND2	1:C:353:ILE:HG13	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:GLY:HA3	1:E:198:PHE:H	1.75	0.50
1:F:79:ILE:HG13	1:F:96:ALA:HB2	1.93	0.50
1:F:269:CYS:HB2	1:F:272:GLY:O	2.11	0.50
1:B:90:ASP:O	1:B:91:GLU:C	2.53	0.50
1:A:297:GLY:HA3	1:B:524:PRO:HD3	1.93	0.50
1:B:11:MET:HG3	1:B:83:TYR:CZ	2.46	0.50
1:E:501:LEU:H	1:E:501:LEU:HD22	1.76	0.50
1:F:115:ALA:N	1:F:116:PRO:CD	2.74	0.50
1:A:64:HIS:CD2	1:A:66:LEU:HB2	2.45	0.50
1:B:400:ARG:HH12	1:B:506:ILE:HG23	1.76	0.50
1:D:6:PHE:CZ	1:D:92:ILE:HD11	2.46	0.50
1:D:600:PHE:O	1:D:601:ARG:HG3	2.12	0.50
1:A:636:ILE:HD12	1:A:636:ILE:N	2.26	0.50
1:B:347:ASP:OD1	2:B:1002:ATP:O2'	2.30	0.50
1:C:9:HIS:CG	1:C:10:ASP:H	2.29	0.50
1:D:400:ARG:HH12	1:D:506:ILE:HG23	1.77	0.50
1:E:109:PRO:HB2	1:E:195:ALA:HB2	1.92	0.50
1:E:489:ARG:HB2	1:E:564:ASN:HD22	1.76	0.50
1:F:539:ASP:OD1	1:F:541:ARG:HG3	2.10	0.50
1:A:545:GLU:O	1:A:549:ARG:HG2	2.12	0.50
1:B:601:ARG:CB	1:B:601:ARG:NH1	2.71	0.50
1:C:238:GLN:NE2	1:C:239:LYS:N	2.60	0.50
1:D:109:PRO:HB2	1:D:195:ALA:HB2	1.94	0.50
1:E:431:SER:HB3	1:E:489:ARG:HG2	1.94	0.50
1:F:64:HIS:O	1:F:68:VAL:HG23	2.12	0.50
1:C:601:ARG:HH11	1:C:601:ARG:HB3	1.77	0.49
1:A:336:LEU:HG	1:A:359:HIS:CD2	2.47	0.49
1:A:436:TYR:HA	1:A:451:LEU:HD22	1.95	0.49
1:B:468:GLN:OE1	1:E:465:VAL:HG21	2.12	0.49
1:D:102:ASN:HD22	1:D:133:HIS:CE1	2.30	0.49
1:E:615:ASP:CG	1:E:616:VAL:N	2.70	0.49
1:B:465:VAL:HG21	1:E:468:GLN:OE1	2.11	0.49
1:C:452:ILE:HG12	1:F:452:ILE:HG12	1.94	0.49
1:D:90:ASP:O	1:D:91:GLU:C	2.55	0.49
1:E:533:GLN:NE2	1:E:533:GLN:N	2.40	0.49
1:A:375:TRP:O	1:A:379:HIS:HD2	1.95	0.49
1:D:615:ASP:CG	1:D:616:VAL:N	2.69	0.49
1:B:233:SER:HB3	1:B:240:PHE:CZ	2.47	0.49
1:E:506:ILE:HG23	1:E:506:ILE:O	2.12	0.49
1:E:601:ARG:CB	1:E:601:ARG:NH1	2.70	0.49
1:F:221:VAL:HG21	1:F:245:SER:CB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ILE:HG23	1:B:506:ILE:O	2.12	0.49
1:C:1:MET:HE1	1:C:98:ALA:CB	2.43	0.49
1:C:114:ARG:O	1:C:115:ALA:HB3	2.11	0.49
1:C:252:SER:C	1:C:254:ALA:H	2.20	0.49
1:D:70:ARG:O	1:D:73:GLN:HB2	2.13	0.49
1:F:78:VAL:HA	1:F:96:ALA:HB1	1.95	0.49
1:F:99:GLY:HA3	1:F:134:ARG:NH1	2.27	0.49
1:E:131:THR:HG23	1:E:144:ILE:HG23	1.93	0.49
1:A:90:ASP:O	1:A:91:GLU:C	2.55	0.49
1:A:347:ASP:OD1	2:A:1001:ATP:O2'	2.31	0.49
1:D:375:TRP:O	1:D:379:HIS:HD2	1.95	0.49
1:D:422:LYS:HD3	1:D:423:TYR:CZ	2.47	0.49
1:F:146:ALA:HB1	1:F:176:THR:HG21	1.93	0.49
1:B:6:PHE:HZ	1:B:92:ILE:HD11	1.78	0.49
1:B:454:GLY:H	1:B:461:TRP:CD1	2.30	0.49
1:C:99:GLY:HA3	1:C:134:ARG:NH1	2.28	0.49
1:C:431:SER:HB3	1:C:489:ARG:CG	2.43	0.49
1:C:454:GLY:H	1:C:461:TRP:CD1	2.30	0.49
1:F:221:VAL:HG21	1:F:245:SER:HB3	1.94	0.49
1:A:79:ILE:HG13	1:A:96:ALA:HB2	1.95	0.49
1:D:426:ARG:HG3	1:D:484:GLN:HG2	1.95	0.49
1:B:1:MET:HE1	1:B:98:ALA:HB2	1.94	0.48
1:B:325:GLY:HA3	2:B:1002:ATP:H5'2	1.95	0.48
1:C:238:GLN:NE2	1:C:239:LYS:H	2.10	0.48
1:C:567:ASN:ND2	1:C:569:GLU:HB2	2.28	0.48
1:E:3:THR:HG22	1:E:78:VAL:CG1	2.42	0.48
1:F:244:SER:HB2	1:F:277:VAL:HB	1.94	0.48
1:A:3:THR:HG22	1:A:78:VAL:CG1	2.42	0.48
1:A:324:ASN:ND2	1:A:353:ILE:HG13	2.26	0.48
1:B:67:TRP:HE1	1:E:604:GLU:CD	2.20	0.48
1:B:545:GLU:O	1:B:549:ARG:HG2	2.13	0.48
1:B:603:VAL:CG1	1:B:607:SER:OG	2.62	0.48
1:C:528:ILE:HD13	3:C:1103:UGA:C2	2.43	0.48
1:D:6:PHE:HZ	1:D:92:ILE:HD11	1.78	0.48
1:A:78:VAL:HA	1:A:96:ALA:HB1	1.94	0.48
1:D:324:ASN:ND2	1:D:353:ILE:HG13	2.28	0.48
1:C:397:GLU:OE2	1:C:400:ARG:NH1	2.46	0.48
1:E:92:ILE:O	1:E:95:LEU:HG	2.13	0.48
1:F:109:PRO:O	1:F:195:ALA:HA	2.12	0.48
1:F:369:ILE:CD1	1:F:390:VAL:HG11	2.43	0.48
1:A:109:PRO:HB2	1:A:195:ALA:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:HIS:CD2	1:B:66:LEU:H	2.31	0.48
1:B:150:ILE:CD1	1:B:165:LEU:HD23	2.44	0.48
1:A:437:GLY:HA3	1:A:452:ILE:O	2.14	0.48
1:A:498:LEU:O	1:A:499:ASP:HB2	2.13	0.48
1:B:431:SER:HB3	1:B:489:ARG:CG	2.44	0.48
1:D:159:ILE:HB	1:D:227:PRO:HD2	1.96	0.48
1:E:109:PRO:O	1:E:195:ALA:HA	2.14	0.48
1:A:533:GLN:NE2	1:A:533:GLN:N	2.41	0.48
1:A:576:GLU:O	1:A:580:MET:HG3	2.14	0.48
1:A:601:ARG:HH11	1:A:601:ARG:HB3	1.77	0.48
1:E:498:LEU:O	1:E:499:ASP:HB2	2.12	0.48
1:F:7:ALA:HB1	1:F:12:GLY:CA	2.43	0.48
1:F:437:GLY:HA3	1:F:452:ILE:O	2.13	0.48
1:A:146:ALA:CB	1:A:176:THR:HG21	2.43	0.48
1:A:228:TRP:HB3	1:A:229:PRO:HD2	1.95	0.48
1:C:11:MET:HG3	1:C:83:TYR:CZ	2.47	0.48
1:C:348:ILE:HG12	2:C:1003:ATP:C2	2.49	0.48
1:D:342:GLU:OE2	1:D:363:HIS:HE1	1.97	0.48
1:D:605:SER:HB2	1:D:613:TYR:CD2	2.49	0.48
1:E:175:GLN:O	1:E:178:PRO:HD2	2.14	0.48
1:A:1:MET:HE1	1:A:98:ALA:HB2	1.94	0.48
1:B:491:PHE:CZ	1:B:621:PRO:HB3	2.49	0.48
1:B:605:SER:HB2	1:B:613:TYR:CD2	2.49	0.48
1:B:636:ILE:HD12	1:B:636:ILE:N	2.25	0.48
1:C:221:VAL:HG21	1:C:245:SER:OG	2.14	0.48
1:A:426:ARG:HG3	1:A:484:GLN:HG2	1.96	0.48
1:B:7:ALA:HB1	1:B:12:GLY:HA2	1.96	0.48
1:C:157:ILE:HG13	1:C:159:ILE:HG22	1.96	0.48
1:C:325:GLY:HA3	2:C:1003:ATP:H5'2	1.95	0.48
1:D:99:GLY:HA3	1:D:134:ARG:NH1	2.29	0.48
1:F:325:GLY:HA3	2:F:1006:ATP:H5'2	1.95	0.48
1:F:399:THR:HG22	1:F:459:PRO:HG2	1.96	0.48
1:F:601:ARG:HH11	1:F:601:ARG:HB2	1.78	0.48
1:A:130:VAL:HG23	1:A:172:LEU:HD13	1.95	0.47
1:A:431:SER:HB3	1:A:489:ARG:CG	2.43	0.47
1:E:600:PHE:O	1:E:601:ARG:HG3	2.14	0.47
1:F:78:VAL:HB	1:F:98:ALA:HB3	1.96	0.47
1:D:64:HIS:CD2	1:D:66:LEU:H	2.32	0.47
1:E:153:ALA:O	1:E:156:ASP:HB2	2.14	0.47
1:F:3:THR:HG22	1:F:78:VAL:CG1	2.42	0.47
1:A:6:PHE:CZ	1:A:92:ILE:HD11	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:SER:C	1:A:254:ALA:N	2.72	0.47
1:C:347:ASP:OD1	2:C:1003:ATP:O2'	2.31	0.47
1:D:108:LEU:HD12	1:D:131:THR:HG21	1.96	0.47
1:D:307:GLN:O	1:D:308:PRO:C	2.57	0.47
1:D:545:GLU:O	1:D:549:ARG:HG2	2.15	0.47
1:E:117:LEU:HD13	1:E:165:LEU:HD12	1.97	0.47
1:A:528:ILE:HD13	3:A:1101:UGA:C2	2.45	0.47
1:B:6:PHE:CZ	1:B:92:ILE:HD11	2.49	0.47
1:B:228:TRP:HB3	1:B:229:PRO:HD2	1.95	0.47
1:C:460:ARG:O	1:C:460:ARG:HG3	2.08	0.47
1:E:375:TRP:O	1:E:379:HIS:HD2	1.96	0.47
1:F:172:LEU:C	1:F:172:LEU:HD23	2.39	0.47
1:B:538:THR:OG1	1:B:566:GLY:HA2	2.14	0.47
1:C:539:ASP:OD1	1:C:541:ARG:HG3	2.15	0.47
1:A:14:LEU:HD12	1:A:15:GLY:N	2.29	0.47
1:A:64:HIS:CD2	1:A:66:LEU:H	2.33	0.47
1:A:64:HIS:ND1	1:A:65:PRO:HD2	2.29	0.47
1:B:277:VAL:HG12	1:B:278:THR:HG23	1.96	0.47
1:D:9:HIS:CG	1:D:10:ASP:H	2.33	0.47
1:D:112:ARG:HH11	1:D:112:ARG:CB	2.28	0.47
1:D:117:LEU:HD13	1:D:165:LEU:HD12	1.96	0.47
1:E:11:MET:HG3	1:E:83:TYR:CZ	2.49	0.47
1:E:150:ILE:HD12	1:E:165:LEU:CD2	2.45	0.47
1:E:430:PRO:HB3	1:E:488:PHE:CZ	2.50	0.47
1:E:567:ASN:ND2	1:E:567:ASN:C	2.72	0.47
1:F:64:HIS:CD2	1:F:66:LEU:H	2.32	0.47
1:F:90:ASP:O	1:F:91:GLU:C	2.57	0.47
1:F:512:ILE:HG23	1:F:513:THR:N	2.30	0.47
1:A:354:SER:HA	1:A:357:LEU:HG	1.97	0.47
1:B:7:ALA:HB1	1:B:12:GLY:CA	2.45	0.47
1:D:109:PRO:O	1:D:195:ALA:HA	2.14	0.47
1:D:334:ARG:NH1	1:D:338:GLU:OE2	2.47	0.47
1:D:501:LEU:HD22	1:D:501:LEU:H	1.80	0.47
1:E:526:LYS:HE3	1:E:603:VAL:HG21	1.96	0.47
1:F:252:SER:C	1:F:254:ALA:N	2.71	0.47
1:A:121:LEU:HD21	1:A:161:LEU:HD22	1.97	0.47
1:A:248:HIS:C	1:A:250:HIS:N	2.72	0.47
1:A:469:LEU:HD12	1:D:469:LEU:HD12	1.97	0.47
1:A:603:VAL:CG1	1:A:607:SER:OG	2.63	0.47
1:B:109:PRO:HB3	1:B:190:GLN:NE2	2.30	0.47
1:B:336:LEU:HG	1:B:359:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:553:ASN:OD1	1:B:558:CYS:HB2	2.15	0.47
1:C:8:TYR:HA	1:C:45:VAL:HG21	1.96	0.47
1:F:119:TRP:CZ2	1:F:201:ARG:HG2	2.50	0.47
1:F:150:ILE:CD1	1:F:165:LEU:HD23	2.45	0.47
1:F:512:ILE:HG23	1:F:513:THR:H	1.80	0.47
1:F:567:ASN:ND2	1:F:569:GLU:HB2	2.28	0.47
1:B:9:HIS:CG	1:B:10:ASP:H	2.33	0.47
1:C:79:ILE:HG13	1:C:96:ALA:HB2	1.97	0.47
1:A:601:ARG:HH11	1:A:601:ARG:HB2	1.76	0.46
1:B:175:GLN:O	1:B:178:PRO:HD2	2.14	0.46
1:B:396:ILE:HD13	1:B:400:ARG:NH2	2.29	0.46
1:C:130:VAL:HG23	1:C:172:LEU:HD13	1.98	0.46
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.48	0.46
1:D:439:CYS:HB3	1:D:444:PHE:CE2	2.50	0.46
1:D:533:GLN:NE2	1:D:533:GLN:N	2.44	0.46
1:E:512:ILE:HG23	1:E:513:THR:N	2.30	0.46
1:F:16:ILE:CD1	1:F:29:ILE:HD13	2.40	0.46
1:F:64:HIS:ND1	1:F:65:PRO:HD2	2.30	0.46
1:F:107:LEU:HD13	1:F:129:GLY:CA	2.45	0.46
1:F:537:PHE:O	1:F:570:ASN:HB2	2.16	0.46
1:C:150:ILE:HD12	1:C:165:LEU:HD23	1.98	0.46
1:D:369:ILE:CD1	1:D:390:VAL:HG11	2.46	0.46
1:E:588:HIS:HD2	1:E:590:LEU:N	2.12	0.46
1:A:369:ILE:CD1	1:A:390:VAL:HG11	2.45	0.46
1:B:211:HIS:O	1:B:270:GLY:HA3	2.14	0.46
1:C:426:ARG:HG3	1:C:484:GLN:HG2	1.96	0.46
1:D:417:ILE:O	1:D:420:CYS:HB2	2.15	0.46
1:E:64:HIS:ND1	1:E:65:PRO:HD2	2.30	0.46
1:E:108:LEU:HD12	1:E:131:THR:CG2	2.46	0.46
1:E:329:ASN:HD22	1:E:355:ARG:HH22	1.61	0.46
1:C:480:LYS:HE2	1:F:400:ARG:O	2.15	0.46
1:D:7:ALA:HB1	1:D:12:GLY:HA2	1.98	0.46
1:E:324:ASN:ND2	1:E:353:ILE:HG13	2.29	0.46
1:E:603:VAL:CG1	1:E:607:SER:OG	2.64	0.46
1:A:406:PHE:O	1:A:410:PHE:HB3	2.16	0.46
1:B:64:HIS:CD2	1:B:66:LEU:HB2	2.45	0.46
1:D:121:LEU:O	1:D:219:ASN:HB3	2.16	0.46
1:E:159:ILE:HG23	1:E:160:THR:N	2.29	0.46
1:B:150:ILE:HD12	1:B:165:LEU:HD23	1.97	0.46
1:D:7:ALA:HB1	1:D:12:GLY:CA	2.45	0.46
1:E:114:ARG:O	1:E:115:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:605:SER:HB2	1:E:613:TYR:CD2	2.50	0.46
1:F:522:GLY:CA	1:F:595:PRO:HG2	2.46	0.46
1:A:99:GLY:HA3	1:A:134:ARG:HH12	1.81	0.46
1:D:314:ARG:HG2	1:D:314:ARG:HH11	1.81	0.46
1:E:7:ALA:HB1	1:E:12:GLY:HA2	1.98	0.46
1:E:437:GLY:HA3	1:E:452:ILE:O	2.16	0.46
1:F:431:SER:HB3	1:F:489:ARG:CG	2.45	0.46
1:A:8:TYR:HA	1:A:45:VAL:HG21	1.98	0.46
1:B:213:PRO:HD2	1:B:216:VAL:HG21	1.98	0.46
1:B:490:PRO:HB3	1:B:493:TRP:CE2	2.50	0.46
1:B:533:GLN:NE2	1:B:533:GLN:N	2.44	0.46
1:C:537:PHE:O	1:C:570:ASN:HB2	2.16	0.46
1:F:114:ARG:O	1:F:115:ALA:HB3	2.16	0.46
1:A:588:HIS:CD2	1:A:590:LEU:HB2	2.50	0.46
1:B:78:VAL:HG23	1:B:99:GLY:O	2.16	0.46
1:E:348:ILE:HG12	2:E:1005:ATP:C2	2.51	0.46
1:A:494:MET:HE1	1:A:642:ILE:HD13	1.97	0.46
1:A:605:SER:HB2	1:A:613:TYR:CD2	2.51	0.46
1:B:157:ILE:HG13	1:B:159:ILE:HG22	1.98	0.46
1:C:553:ASN:OD1	1:C:558:CYS:HB2	2.15	0.46
1:D:157:ILE:HG13	1:D:159:ILE:HG22	1.98	0.46
1:D:201:ARG:HH22	1:D:220:MET:HE1	1.80	0.46
1:E:79:ILE:HG13	1:E:96:ALA:HB2	1.98	0.46
1:F:109:PRO:HB2	1:F:195:ALA:CB	2.46	0.46
1:F:582:LEU:HD11	1:F:597:PHE:CE2	2.51	0.46
1:A:159:ILE:HB	1:A:227:PRO:HD2	1.99	0.45
1:A:210:TRP:HA	1:A:217:LEU:HD11	1.97	0.45
1:B:157:ILE:O	1:B:158:ALA:C	2.60	0.45
1:D:150:ILE:HD12	1:D:165:LEU:HD23	1.98	0.45
1:D:325:GLY:HA3	2:D:1004:ATP:H5'2	1.98	0.45
1:E:90:ASP:O	1:E:91:GLU:C	2.58	0.45
1:A:396:ILE:HD13	1:A:400:ARG:NH2	2.31	0.45
1:B:287:MET:HA	1:F:50:ALA:HB2	1.99	0.45
1:B:375:TRP:O	1:B:379:HIS:HD2	1.98	0.45
1:C:213:PRO:HD2	1:C:216:VAL:CG2	2.46	0.45
1:C:336:LEU:HD21	1:C:362:PHE:HB2	1.97	0.45
1:D:506:ILE:O	1:D:506:ILE:CG2	2.64	0.45
1:F:7:ALA:HB1	1:F:12:GLY:HA2	1.98	0.45
1:A:392:ILE:HG13	1:A:408:LEU:HD12	1.98	0.45
1:A:468:GLN:OE1	1:D:465:VAL:HG21	2.16	0.45
1:C:252:SER:C	1:C:254:ALA:N	2.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:TYR:HA	1:D:45:VAL:HG21	1.97	0.45
1:D:110:LYS:NZ	1:D:194:GLU:HB3	2.31	0.45
1:D:211:HIS:O	1:D:270:GLY:HA3	2.17	0.45
1:E:392:ILE:HG13	1:E:408:LEU:HD12	1.98	0.45
1:F:6:PHE:O	1:F:84:TYR:HB2	2.16	0.45
1:F:88:ILE:HG22	1:F:93:LEU:CD2	2.46	0.45
1:A:90:ASP:O	1:A:94:GLN:HG2	2.16	0.45
1:C:19:LEU:HD11	1:C:80:PHE:CE2	2.51	0.45
1:C:314:ARG:HG2	1:C:314:ARG:HH11	1.82	0.45
1:C:399:THR:HG22	1:C:459:PRO:HG2	1.99	0.45
1:D:107:LEU:HD13	1:D:129:GLY:CA	2.47	0.45
1:E:201:ARG:HH22	1:E:220:MET:HE1	1.81	0.45
1:E:406:PHE:O	1:E:410:PHE:HB3	2.16	0.45
1:F:636:ILE:H	1:F:636:ILE:CD1	2.28	0.45
1:A:50:ALA:HB2	1:E:287:MET:HA	1.99	0.45
1:B:530:GLY:H	1:B:602:VAL:HG13	1.81	0.45
1:C:400:ARG:O	1:F:480:LYS:HE2	2.16	0.45
1:D:228:TRP:HB3	1:D:229:PRO:HD2	1.97	0.45
1:D:528:ILE:HD13	3:D:1104:UGA:C2	2.45	0.45
1:E:348:ILE:HD13	1:E:367:GLY:O	2.17	0.45
1:F:514:GLN:NE2	1:F:608:TYR:OH	2.41	0.45
1:B:102:ASN:HD22	1:B:133:HIS:CE1	2.35	0.45
1:B:114:ARG:O	1:B:115:ALA:HB3	2.16	0.45
1:D:108:LEU:HD12	1:D:131:THR:CG2	2.47	0.45
1:D:489:ARG:HB2	1:D:564:ASN:HD22	1.81	0.45
1:D:601:ARG:HH11	1:D:601:ARG:HB2	1.80	0.45
1:E:159:ILE:HB	1:E:227:PRO:HD2	1.99	0.45
1:E:252:SER:O	1:E:254:ALA:N	2.50	0.45
1:E:353:ILE:C	1:E:353:ILE:HD12	2.42	0.45
1:F:567:ASN:HD22	1:F:569:GLU:H	1.65	0.45
1:A:539:ASP:OD1	1:A:541:ARG:HG3	2.17	0.45
1:C:109:PRO:O	1:C:195:ALA:HA	2.16	0.45
1:E:512:ILE:HG23	1:E:513:THR:H	1.81	0.45
1:F:498:LEU:O	1:F:499:ASP:HB2	2.17	0.45
1:D:119:TRP:CZ2	1:D:201:ARG:HG2	2.51	0.45
1:D:338:GLU:HG3	1:D:548:TYR:OH	2.16	0.45
1:F:102:ASN:HD22	1:F:133:HIS:CE1	2.34	0.45
1:A:403:LEU:O	1:A:407:GLU:HG3	2.17	0.45
1:D:348:ILE:HG12	2:D:1004:ATP:C2	2.52	0.45
1:D:436:TYR:HA	1:D:451:LEU:HD22	1.98	0.45
1:F:434:GLU:OE2	1:F:460:ARG:NH2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:515:LEU:HA	1:F:518:ASN:ND2	2.28	0.45
1:A:348:ILE:HG12	2:A:1001:ATP:C2	2.51	0.45
1:B:107:LEU:HD13	1:B:129:GLY:CA	2.47	0.45
1:C:512:ILE:HG23	1:C:513:THR:N	2.32	0.45
1:D:252:SER:C	1:D:254:ALA:H	2.25	0.45
1:E:9:HIS:CG	1:E:10:ASP:H	2.34	0.45
1:F:538:THR:OG1	1:F:566:GLY:HA2	2.17	0.45
1:B:582:LEU:HD11	1:B:597:PHE:CE2	2.52	0.44
1:F:347:ASP:OD1	2:F:1006:ATP:O2'	2.33	0.44
1:C:1:MET:HE1	1:C:98:ALA:HB2	1.99	0.44
1:C:16:ILE:HD13	1:C:29:ILE:CD1	2.39	0.44
1:C:359:HIS:HA	1:C:360:PRO:HD3	1.87	0.44
1:C:396:ILE:HD13	1:C:400:ARG:NH2	2.32	0.44
1:D:146:ALA:CB	1:D:176:THR:HG21	2.47	0.44
1:D:235:VAL:HG23	1:D:240:PHE:CE1	2.53	0.44
1:E:325:GLY:HA3	2:E:1005:ATP:H5'2	1.99	0.44
1:F:8:TYR:HA	1:F:45:VAL:HG21	1.99	0.44
1:F:121:LEU:HD21	1:F:161:LEU:HD22	1.98	0.44
1:F:233:SER:HB3	1:F:240:PHE:CZ	2.51	0.44
1:A:119:TRP:CZ2	1:A:201:ARG:HG2	2.51	0.44
1:A:567:ASN:HD21	1:A:569:GLU:HB2	1.83	0.44
1:C:12:GLY:O	1:C:16:ILE:HG13	2.17	0.44
1:C:146:ALA:CB	1:C:176:THR:HG21	2.47	0.44
1:B:78:VAL:HG22	1:B:79:ILE:N	2.32	0.44
1:E:110:LYS:NZ	1:E:194:GLU:HB3	2.33	0.44
1:F:201:ARG:HH22	1:F:220:MET:HE1	1.83	0.44
1:A:334:ARG:NH1	1:A:338:GLU:OE2	2.51	0.44
1:B:567:ASN:ND2	1:B:567:ASN:C	2.76	0.44
1:C:146:ALA:HB1	1:C:176:THR:HG21	2.00	0.44
1:D:201:ARG:NH2	1:D:220:MET:HE1	2.33	0.44
1:E:235:VAL:HG23	1:E:240:PHE:CE1	2.53	0.44
1:F:364:PHE:CG	1:F:365:VAL:N	2.86	0.44
1:B:326:PHE:CZ	1:B:540:ILE:HD13	2.52	0.44
1:C:113:GLY:HA3	1:C:198:PHE:O	2.18	0.44
1:C:299:VAL:O	1:C:301:GLY:N	2.46	0.44
1:D:399:THR:HG22	1:D:459:PRO:HG2	2.00	0.44
1:D:539:ASP:OD1	1:D:541:ARG:HG3	2.17	0.44
1:E:70:ARG:O	1:E:73:GLN:HB2	2.17	0.44
1:E:334:ARG:NH1	1:E:338:GLU:OE2	2.51	0.44
1:C:436:TYR:HA	1:C:451:LEU:HD22	1.99	0.44
1:C:501:LEU:H	1:C:501:LEU:HD22	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:567:ASN:C	1:C:567:ASN:ND2	2.76	0.44
1:F:14:LEU:HD12	1:F:14:LEU:C	2.41	0.44
1:A:510:ARG:NH1	2:A:1001:ATP:O3G	2.51	0.44
1:C:534:LYS:HA	1:C:573:SER:HA	1.99	0.44
1:D:11:MET:HG3	1:D:83:TYR:CZ	2.52	0.44
1:D:12:GLY:O	1:D:16:ILE:HG13	2.18	0.44
1:F:243:TRP:CD1	1:F:279:GLY:HA2	2.53	0.44
1:F:436:TYR:HA	1:F:451:LEU:HD22	1.99	0.44
1:F:567:ASN:ND2	1:F:567:ASN:C	2.74	0.44
1:A:235:VAL:HG23	1:A:240:PHE:CE1	2.53	0.44
1:B:485:PHE:CZ	1:B:560:GLY:HA2	2.52	0.44
1:B:594:PHE:HB3	1:B:595:PRO:HD2	2.00	0.44
1:C:524:PRO:HB2	1:C:601:ARG:HD3	2.00	0.44
1:C:545:GLU:O	1:C:549:ARG:HG2	2.16	0.44
1:D:522:GLY:CA	1:D:595:PRO:HG2	2.48	0.44
1:E:403:LEU:O	1:E:407:GLU:HG3	2.18	0.44
1:F:603:VAL:CG1	1:F:607:SER:OG	2.65	0.44
1:A:157:ILE:HG13	1:A:159:ILE:HG22	1.99	0.43
1:A:159:ILE:HG23	1:A:160:THR:N	2.33	0.43
1:A:424:ARG:HG2	1:A:424:ARG:NH1	2.32	0.43
1:A:489:ARG:HB2	1:A:564:ASN:HD22	1.83	0.43
1:B:146:ALA:HB1	1:B:176:THR:HG21	2.00	0.43
1:B:359:HIS:HA	1:B:360:PRO:HD3	1.88	0.43
1:B:399:THR:HG22	1:B:459:PRO:HG2	2.00	0.43
1:B:424:ARG:HG2	1:B:424:ARG:NH1	2.33	0.43
1:C:392:ILE:HG13	1:C:408:LEU:HD12	2.00	0.43
1:D:78:VAL:HA	1:D:96:ALA:HB1	1.99	0.43
1:D:156:ASP:O	1:D:222:ARG:HD2	2.18	0.43
1:E:107:LEU:HD13	1:E:129:GLY:CA	2.48	0.43
1:B:338:GLU:HB3	1:B:340:HIS:CE1	2.52	0.43
1:B:522:GLY:CA	1:B:595:PRO:HG2	2.48	0.43
1:F:314:ARG:HG2	1:F:314:ARG:HH11	1.83	0.43
1:F:369:ILE:HD11	1:F:390:VAL:HG11	1.99	0.43
1:A:364:PHE:CG	1:A:365:VAL:N	2.86	0.43
1:B:16:ILE:CD1	1:B:29:ILE:HD13	2.40	0.43
1:B:252:SER:O	1:B:254:ALA:N	2.50	0.43
1:B:437:GLY:HA3	1:B:452:ILE:O	2.19	0.43
1:D:159:ILE:HG23	1:D:160:THR:N	2.33	0.43
1:D:353:ILE:HD12	1:D:353:ILE:C	2.43	0.43
1:E:221:VAL:HG21	1:E:245:SER:HB3	2.01	0.43
1:E:485:PHE:CD1	1:E:485:PHE:C	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:582:LEU:HD11	1:E:597:PHE:CE2	2.54	0.43
1:F:130:VAL:HG23	1:F:172:LEU:HD13	1.99	0.43
1:F:190:GLN:O	1:F:192:GLU:N	2.51	0.43
1:F:590:LEU:HD11	1:F:651:ARG:NH1	2.33	0.43
1:F:600:PHE:O	1:F:601:ARG:HG3	2.18	0.43
1:A:400:ARG:HH12	1:A:506:ILE:HG23	1.83	0.43
1:B:119:TRP:CZ2	1:B:201:ARG:HG2	2.54	0.43
1:B:348:ILE:HD13	1:B:367:GLY:O	2.19	0.43
1:B:567:ASN:ND2	1:B:569:GLU:HB2	2.33	0.43
1:C:259:VAL:HG22	1:C:267:ILE:CD1	2.48	0.43
1:C:354:SER:HA	1:C:357:LEU:HG	2.00	0.43
1:C:601:ARG:HH11	1:C:601:ARG:HB2	1.78	0.43
1:E:89:TYR:O	1:E:90:ASP:C	2.61	0.43
1:E:248:HIS:C	1:E:250:HIS:N	2.74	0.43
1:A:14:LEU:HD12	1:A:14:LEU:C	2.43	0.43
1:A:314:ARG:HG2	1:A:314:ARG:HH11	1.84	0.43
1:B:485:PHE:CD1	1:B:485:PHE:C	2.97	0.43
1:D:246:ARG:HB3	1:D:275:GLU:HB3	2.01	0.43
1:E:157:ILE:O	1:E:158:ALA:C	2.61	0.43
1:E:157:ILE:HG13	1:E:159:ILE:HG22	1.99	0.43
1:E:248:HIS:C	1:E:250:HIS:H	2.26	0.43
1:A:16:ILE:CD1	1:A:29:ILE:HD13	2.44	0.43
1:A:109:PRO:HB3	1:A:190:GLN:NE2	2.33	0.43
1:B:336:LEU:HD12	1:B:336:LEU:HA	1.88	0.43
1:C:87:LEU:HD12	1:C:88:ILE:N	2.34	0.43
1:D:248:HIS:C	1:D:250:HIS:N	2.76	0.43
1:F:324:ASN:ND2	1:F:353:ILE:HG13	2.31	0.43
1:B:348:ILE:HG12	2:B:1002:ATP:C2	2.54	0.43
1:B:392:ILE:HG13	1:B:408:LEU:HD12	2.00	0.43
1:C:64:HIS:ND1	1:C:65:PRO:HD2	2.33	0.43
1:C:78:VAL:HA	1:C:96:ALA:HB1	2.00	0.43
1:C:522:GLY:CA	1:C:595:PRO:HG2	2.49	0.43
1:C:576:GLU:O	1:C:580:MET:HG3	2.18	0.43
1:F:546:ALA:HB3	1:F:565:ILE:HD13	2.00	0.43
1:A:538:THR:OG1	1:A:566:GLY:HA2	2.19	0.43
1:B:99:GLY:HA3	1:B:134:ARG:NH1	2.33	0.43
1:C:492:ASN:OD1	1:C:535:ARG:HD2	2.18	0.43
1:D:150:ILE:CD1	1:D:165:LEU:HD23	2.49	0.43
1:F:213:PRO:HB2	1:F:216:VAL:HG23	2.00	0.43
1:B:369:ILE:HD11	1:B:390:VAL:HG11	2.00	0.43
1:B:539:ASP:OD1	1:B:541:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ASP:OD1	2:D:1004:ATP:O2'	2.35	0.43
1:B:601:ARG:HB3	1:B:601:ARG:NH1	2.34	0.43
1:C:221:VAL:HG21	1:C:245:SER:CB	2.49	0.43
1:C:636:ILE:H	1:C:636:ILE:CD1	2.30	0.43
1:D:582:LEU:HD11	1:D:597:PHE:CE2	2.53	0.43
1:E:221:VAL:HG21	1:E:245:SER:CB	2.49	0.43
1:E:233:SER:HB3	1:E:240:PHE:CZ	2.54	0.43
1:E:369:ILE:HD11	1:E:390:VAL:HG11	2.00	0.43
1:F:110:LYS:NZ	1:F:194:GLU:HB3	2.33	0.43
1:F:354:SER:HA	1:F:357:LEU:HG	2.01	0.43
1:A:490:PRO:HB3	1:A:493:TRP:CE2	2.53	0.42
1:A:506:ILE:O	1:A:506:ILE:CG2	2.66	0.42
1:B:1:MET:HE2	1:B:77:ASP:CB	2.47	0.42
1:F:15:GLY:O	1:F:19:LEU:HB2	2.19	0.42
1:F:430:PRO:HB3	1:F:488:PHE:CZ	2.54	0.42
1:B:117:LEU:HD13	1:B:165:LEU:HD12	2.01	0.42
1:B:510:ARG:NH1	2:B:1002:ATP:O3G	2.52	0.42
1:C:375:TRP:O	1:C:379:HIS:HD2	2.01	0.42
1:A:362:PHE:CE2	1:A:364:PHE:HB2	2.55	0.42
1:A:524:PRO:HB2	1:A:601:ARG:HD3	2.00	0.42
1:C:133:HIS:HD2	1:C:134:ARG:O	2.01	0.42
1:D:329:ASN:HD22	1:D:355:ARG:HH22	1.64	0.42
1:D:567:ASN:C	1:D:567:ASN:ND2	2.77	0.42
1:F:221:VAL:HG21	1:F:245:SER:OG	2.19	0.42
1:C:78:VAL:HG23	1:C:99:GLY:O	2.19	0.42
1:D:490:PRO:HB3	1:D:493:TRP:CE2	2.54	0.42
1:D:588:HIS:CG	1:D:589:PRO:HD2	2.54	0.42
1:E:99:GLY:HA3	1:E:134:ARG:NH1	2.35	0.42
1:E:315:ARG:CZ	1:E:361:HIS:NE2	2.83	0.42
1:B:107:LEU:CD1	1:B:129:GLY:HA3	2.50	0.42
1:B:159:ILE:HG23	1:B:160:THR:N	2.34	0.42
1:C:111:TYR:H	1:C:196:THR:HB	1.85	0.42
1:F:528:ILE:HD13	3:F:1106:UGA:C2	2.49	0.42
1:C:533:GLN:NE2	1:C:533:GLN:N	2.42	0.42
1:D:330:HIS:HB3	1:D:544:ILE:HG12	2.02	0.42
1:F:69:GLU:O	1:F:72:ALA:HB3	2.20	0.42
1:F:524:PRO:HB2	1:F:601:ARG:HD3	2.01	0.42
1:A:7:ALA:HB1	1:A:12:GLY:CA	2.50	0.42
1:A:78:VAL:HG22	1:A:79:ILE:N	2.35	0.42
1:A:107:LEU:HD13	1:A:129:GLY:CA	2.49	0.42
1:A:329:ASN:ND2	1:A:355:ARG:NH2	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:109:PRO:HB3	1:C:190:GLN:NE2	2.34	0.42
1:C:150:ILE:CD1	1:C:165:LEU:HD23	2.49	0.42
1:C:177:LEU:HD12	1:C:177:LEU:HA	1.92	0.42
1:C:540:ILE:CD1	1:C:544:ILE:HD13	2.50	0.42
1:D:221:VAL:HG21	1:D:245:SER:CB	2.49	0.42
1:D:336:LEU:HD21	1:D:362:PHE:HB2	2.02	0.42
1:D:431:SER:HB3	1:D:489:ARG:CG	2.50	0.42
1:E:109:PRO:HB3	1:E:190:GLN:NE2	2.35	0.42
1:E:336:LEU:HD12	1:E:336:LEU:HA	1.90	0.42
1:E:342:GLU:OE2	1:E:363:HIS:HE1	2.01	0.42
1:F:155:ASP:OD1	1:F:155:ASP:N	2.52	0.42
1:B:489:ARG:HB2	1:B:564:ASN:HD22	1.84	0.42
1:D:112:ARG:HH22	1:D:190:GLN:NE2	2.18	0.42
1:E:201:ARG:NH2	1:E:220:MET:HE1	2.35	0.42
1:E:485:PHE:CZ	1:E:560:GLY:HA2	2.54	0.42
1:A:228:TRP:CB	1:A:229:PRO:HD2	2.50	0.42
1:A:534:LYS:HA	1:A:573:SER:HA	2.02	0.42
1:B:362:PHE:CE2	1:B:364:PHE:HB2	2.55	0.42
1:C:131:THR:HG23	1:C:144:ILE:HG23	2.02	0.42
1:C:416:ILE:N	1:C:416:ILE:HD12	2.35	0.42
1:D:636:ILE:H	1:D:636:ILE:CD1	2.28	0.42
1:E:146:ALA:CB	1:E:176:THR:HG21	2.49	0.42
1:E:228:TRP:HB3	1:E:229:PRO:HD2	2.00	0.42
1:E:491:PHE:CE2	1:E:621:PRO:HB3	2.55	0.42
1:F:336:LEU:HD12	1:F:336:LEU:HA	1.85	0.42
1:C:567:ASN:HD22	1:C:569:GLU:H	1.66	0.42
1:D:327:ILE:HD11	2:D:1004:ATP:O2G	2.20	0.42
1:E:7:ALA:HB1	1:E:12:GLY:CA	2.50	0.42
1:E:112:ARG:CB	1:E:112:ARG:HH11	2.33	0.42
1:E:314:ARG:HG2	1:E:314:ARG:HH11	1.83	0.42
1:F:159:ILE:HB	1:F:227:PRO:HD2	2.01	0.42
1:F:406:PHE:O	1:F:410:PHE:HB3	2.20	0.42
1:F:435:VAL:HG22	1:F:468:GLN:HB2	2.01	0.42
1:A:430:PRO:HB3	1:A:488:PHE:CZ	2.55	0.41
1:A:458:LYS:HD3	1:A:458:LYS:HA	1.92	0.41
1:B:436:TYR:HA	1:B:451:LEU:HD22	2.02	0.41
1:D:603:VAL:CG1	1:D:607:SER:OG	2.68	0.41
1:E:246:ARG:HB3	1:E:275:GLU:HB3	2.02	0.41
1:F:398:TYR:CD1	1:F:398:TYR:N	2.87	0.41
1:A:400:ARG:O	1:D:480:LYS:HE2	2.19	0.41
1:B:314:ARG:NH1	1:B:315:ARG:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:TYR:O	1:C:90:ASP:C	2.62	0.41
1:C:605:SER:HB2	1:C:613:TYR:CD2	2.56	0.41
1:D:31:THR:HG23	1:D:32:HIS:N	2.35	0.41
1:D:155:ASP:OD1	1:D:155:ASP:N	2.49	0.41
1:D:213:PRO:HB2	1:D:216:VAL:HG23	2.02	0.41
1:E:71:ILE:HD12	1:E:92:ILE:HD12	2.02	0.41
1:F:4:VAL:HG23	1:F:76:PRO:HB3	2.02	0.41
1:F:601:ARG:HH11	1:F:601:ARG:HB3	1.84	0.41
1:C:226:ASP:CG	1:C:227:PRO:HA	2.45	0.41
1:D:111:TYR:CE2	1:D:120:VAL:HG12	2.55	0.41
1:D:228:TRP:CB	1:D:229:PRO:HD2	2.51	0.41
1:D:354:SER:HA	1:D:357:LEU:HG	2.01	0.41
1:E:69:GLU:O	1:E:73:GLN:HG2	2.20	0.41
1:E:190:GLN:O	1:E:192:GLU:N	2.53	0.41
1:E:238:GLN:NE2	1:E:239:LYS:H	2.18	0.41
1:E:528:ILE:HD13	3:E:1105:UGA:C2	2.50	0.41
1:E:541:ARG:HH12	1:E:636:ILE:HG12	1.85	0.41
1:F:353:ILE:HD12	1:F:353:ILE:C	2.45	0.41
1:C:506:ILE:O	1:C:506:ILE:HG23	2.19	0.41
1:D:524:PRO:HB2	1:D:601:ARG:HD3	2.00	0.41
1:F:113:GLY:HA3	1:F:198:PHE:O	2.21	0.41
1:F:582:LEU:HD11	1:F:597:PHE:CD2	2.56	0.41
1:F:588:HIS:HD2	1:F:590:LEU:N	2.11	0.41
1:A:110:LYS:NZ	1:A:194:GLU:HB3	2.35	0.41
1:A:157:ILE:O	1:A:158:ALA:C	2.63	0.41
1:B:221:VAL:HG21	1:B:245:SER:CB	2.50	0.41
1:C:121:LEU:O	1:C:219:ASN:HB3	2.21	0.41
1:E:522:GLY:CA	1:E:595:PRO:HG2	2.50	0.41
1:E:588:HIS:HA	1:E:589:PRO:HD3	1.94	0.41
1:F:111:TYR:CE2	1:F:120:VAL:HG12	2.55	0.41
1:F:296:LEU:CB	1:F:298:LEU:HD13	2.50	0.41
1:F:485:PHE:CZ	1:F:560:GLY:HA2	2.55	0.41
1:A:327:ILE:HD11	2:A:1001:ATP:O2G	2.21	0.41
1:B:129:GLY:HA2	1:B:150:ILE:HD12	2.02	0.41
1:B:430:PRO:HB3	1:B:488:PHE:CZ	2.54	0.41
1:B:511:ALA:O	1:B:512:ILE:C	2.62	0.41
1:D:406:PHE:O	1:D:410:PHE:HB3	2.20	0.41
1:D:594:PHE:HB3	1:D:595:PRO:HD2	2.03	0.41
1:E:400:ARG:HH12	1:E:506:ILE:HG23	1.86	0.41
1:F:435:VAL:CG2	1:F:468:GLN:HB2	2.51	0.41
1:A:1:MET:H3	1:A:181:LYS:HE3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:GLU:OE2	1:A:363:HIS:HE1	2.02	0.41
1:B:113:GLY:HA3	1:B:198:PHE:O	2.20	0.41
1:C:437:GLY:HA3	1:C:452:ILE:O	2.21	0.41
1:D:159:ILE:O	1:D:162:HIS:HB3	2.21	0.41
1:D:546:ALA:HB3	1:D:565:ILE:HD13	2.03	0.41
1:F:130:VAL:HG23	1:F:172:LEU:CD1	2.50	0.41
1:F:534:LYS:HA	1:F:573:SER:HA	2.03	0.41
1:A:221:VAL:HG21	1:A:245:SER:CB	2.51	0.41
1:A:243:TRP:CD1	1:A:279:GLY:HA2	2.55	0.41
1:B:217:LEU:HD12	1:B:269:CYS:SG	2.61	0.41
1:C:512:ILE:HG23	1:C:513:THR:H	1.85	0.41
1:E:5:VAL:HG21	1:E:19:LEU:HD23	2.01	0.41
1:E:77:ASP:O	1:E:98:ALA:HB3	2.21	0.41
1:E:90:ASP:O	1:E:94:GLN:HG2	2.20	0.41
1:A:69:GLU:O	1:A:73:GLN:HG2	2.21	0.41
1:A:580:MET:HE3	1:A:639:GLN:NE2	2.36	0.41
1:B:491:PHE:CE1	1:B:621:PRO:HB3	2.55	0.41
1:B:506:ILE:O	1:B:506:ILE:CG2	2.69	0.41
1:C:107:LEU:HD13	1:C:129:GLY:CA	2.50	0.41
1:C:373:SER:O	1:C:374:GLU:C	2.63	0.41
1:D:131:THR:HG23	1:D:144:ILE:HG23	2.02	0.41
1:E:113:GLY:HA3	1:E:198:PHE:O	2.20	0.41
1:E:636:ILE:HD12	1:E:636:ILE:N	2.29	0.41
1:F:338:GLU:HB3	1:F:340:HIS:CE1	2.56	0.41
1:F:522:GLY:HA3	1:F:595:PRO:CG	2.50	0.41
1:A:112:ARG:NH1	1:A:140:ASP:O	2.54	0.41
1:A:492:ASN:OD1	1:A:535:ARG:HD2	2.21	0.41
1:B:90:ASP:O	1:B:94:GLN:HG2	2.21	0.41
1:B:214:ALA:HB1	1:B:247:VAL:HG12	2.03	0.41
1:B:431:SER:CB	1:B:489:ARG:HG2	2.51	0.41
1:B:506:ILE:HD12	1:B:506:ILE:HA	1.89	0.41
1:C:233:SER:HB3	1:C:240:PHE:CZ	2.56	0.41
1:C:336:LEU:HG	1:C:359:HIS:CD2	2.56	0.41
1:D:88:ILE:H	1:D:88:ILE:HG13	1.76	0.41
1:D:157:ILE:O	1:D:158:ALA:C	2.64	0.41
1:E:398:TYR:CD1	1:E:398:TYR:N	2.88	0.41
1:C:159:ILE:HG23	1:C:160:THR:N	2.36	0.40
1:C:538:THR:OG1	1:C:566:GLY:HA2	2.21	0.40
1:D:392:ILE:HG13	1:D:408:LEU:HD12	2.03	0.40
1:E:1:MET:HE2	1:E:77:ASP:CB	2.42	0.40
1:E:590:LEU:HD11	1:E:651:ARG:NH1	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:601:ARG:NH2	1:F:295:THR:HA	2.36	0.40
1:F:8:TYR:CA	1:F:45:VAL:HG21	2.51	0.40
1:F:359:HIS:HA	1:F:360:PRO:HD3	1.91	0.40
1:A:94:GLN:HG2	1:A:94:GLN:H	1.63	0.40
1:A:107:LEU:HD12	1:A:107:LEU:HA	1.89	0.40
1:A:397:GLU:OE2	1:A:400:ARG:NH1	2.54	0.40
1:A:588:HIS:HD2	1:A:590:LEU:HB2	1.85	0.40
1:B:435:VAL:CG2	1:B:468:GLN:HB2	2.51	0.40
1:B:588:HIS:HA	1:B:589:PRO:HD3	1.98	0.40
1:D:8:TYR:CA	1:D:45:VAL:HG21	2.52	0.40
1:D:111:TYR:H	1:D:196:THR:HB	1.86	0.40
1:D:398:TYR:N	1:D:398:TYR:CD1	2.90	0.40
1:D:537:PHE:O	1:D:570:ASN:HB2	2.21	0.40
1:F:101:PHE:CE2	1:F:145:VAL:HG21	2.56	0.40
1:F:317:ARG:HG3	1:F:317:ARG:NH1	2.37	0.40
1:A:373:SER:O	1:A:374:GLU:C	2.64	0.40
1:B:10:ASP:O	1:B:11:MET:C	2.64	0.40
1:B:315:ARG:CZ	1:B:361:HIS:NE2	2.84	0.40
1:B:364:PHE:CG	1:B:365:VAL:N	2.89	0.40
1:B:375:TRP:CE2	1:B:379:HIS:CD2	3.09	0.40
1:C:109:PRO:HB2	1:C:195:ALA:HB2	2.04	0.40
1:C:353:ILE:C	1:C:353:ILE:HD12	2.46	0.40
1:F:232:PHE:CG	1:F:239:LYS:HE3	2.56	0.40
1:A:248:HIS:C	1:A:250:HIS:H	2.30	0.40
1:A:359:HIS:HA	1:A:360:PRO:HD3	1.89	0.40
1:C:434:GLU:OE2	1:C:460:ARG:NH2	2.55	0.40
1:C:603:VAL:CG1	1:C:607:SER:OG	2.69	0.40
1:D:416:ILE:N	1:D:416:ILE:HD12	2.37	0.40
1:D:470:LEU:HD23	1:D:470:LEU:HA	1.97	0.40
1:E:10:ASP:O	1:E:11:MET:C	2.64	0.40
1:E:367:GLY:HA2	1:E:372:HIS:CD2	2.57	0.40
1:E:397:GLU:OE2	1:E:400:ARG:NH1	2.53	0.40
1:E:424:ARG:HG2	1:E:424:ARG:NH1	2.36	0.40
1:E:490:PRO:HB3	1:E:493:TRP:CE2	2.57	0.40
1:F:121:LEU:HD13	1:F:121:LEU:HA	1.95	0.40
1:F:136:VAL:HG22	1:F:142:GLY:H	1.85	0.40
1:A:7:ALA:HB1	1:A:12:GLY:HA2	2.04	0.40
1:A:112:ARG:CB	1:A:112:ARG:HH11	2.34	0.40
1:A:391:ALA:HA	1:A:408:LEU:HD13	2.04	0.40
1:A:594:PHE:HB3	1:A:595:PRO:HD2	2.03	0.40
1:C:314:ARG:NH1	1:C:315:ARG:O	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LEU:HA	1:C:336:LEU:HD12	1.76	0.40
1:C:367:GLY:HA2	1:C:372:HIS:CD2	2.56	0.40
1:C:390:VAL:HG13	2:C:1003:ATP:C4	2.57	0.40
1:D:102:ASN:HD22	1:D:133:HIS:HE1	1.69	0.40
1:E:299:VAL:O	1:E:301:GLY:N	2.54	0.40

All (2) 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:B:184:ASN:ND2	1:C:171:GLN:OE1[1_655]	2.03	0.17
1:B:182:HIS:O	1:C:167:HIS:NE2[1_655]	2.13	0.07

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	633/660 (96%)	581 (92%)	42 (7%)	10 (2%)	7	34
1	B	633/660 (96%)	578 (91%)	43 (7%)	12 (2%)	6	30
1	C	633/660 (96%)	573 (90%)	50 (8%)	10 (2%)	7	34
1	D	638/660 (97%)	584 (92%)	44 (7%)	10 (2%)	7	34
1	E	633/660 (96%)	580 (92%)	42 (7%)	11 (2%)	7	32
1	F	633/660 (96%)	577 (91%)	45 (7%)	11 (2%)	7	32
All	All	3803/3960 (96%)	3473 (91%)	266 (7%)	64 (2%)	7	32

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	ASP
1	A	300	GLN

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Mol	Chain	Res	Type
1	A	302	SER
1	B	90	ASP
1	B	251	ALA
1	B	302	SER
1	C	90	ASP
1	D	90	ASP
1	E	90	ASP
1	F	90	ASP
1	F	142	GLY
1	F	302	SER
1	A	142	GLY
1	B	250	HIS
1	C	142	GLY
1	C	302	SER
1	D	142	GLY
1	D	189	ALA
1	F	189	ALA
1	A	210	TRP
1	A	250	HIS
1	B	142	GLY
1	C	250	HIS
1	C	251	ALA
1	C	300	GLN
1	D	250	HIS
1	D	302	SER
1	E	253	LYS
1	E	300	GLN
1	E	302	SER
1	F	191	ARG
1	F	250	HIS
1	A	183	GLY
1	A	251	ALA
1	B	253	LYS
1	E	192	GLU
1	E	251	ALA
1	E	252	SER
1	F	192	GLU
1	F	251	ALA
1	A	253	LYS
1	B	246	ARG
1	B	252	SER
1	B	300	GLN

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Mol	Chain	Res	Type
1	C	91	GLU
1	C	192	GLU
1	D	188	ILE
1	D	246	ARG
1	E	183	GLY
1	E	191	ARG
1	F	113	GLY
1	F	188	ILE
1	A	113	GLY
1	B	431	SER
1	D	113	GLY
1	E	210	TRP
1	F	183	GLY
1	B	183	GLY
1	C	113	GLY
1	D	115	ALA
1	E	113	GLY
1	B	113	GLY
1	C	183	GLY
1	D	299	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	526/559 (94%)	491 (93%)	35 (7%)	15	46
1	B	526/559 (94%)	490 (93%)	36 (7%)	14	45
1	C	526/559 (94%)	489 (93%)	37 (7%)	14	44
1	D	528/559 (94%)	493 (93%)	35 (7%)	15	46
1	E	526/559 (94%)	491 (93%)	35 (7%)	15	46
1	F	526/559 (94%)	488 (93%)	38 (7%)	13	43
All	All	3158/3354 (94%)	2942 (93%)	216 (7%)	14	45

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	ASP
1	A	89	TYR
1	A	91	GLU
1	A	92	ILE
1	A	103	LEU
1	A	107	LEU
1	A	112	ARG
1	A	121	LEU
1	A	125	GLU
1	A	164	LYS
1	A	221	VAL
1	A	304	LEU
1	A	314	ARG
1	A	319	LEU
1	A	336	LEU
1	A	385	VAL
1	A	387	LEU
1	A	408	LEU
1	A	421	VAL
1	A	435	VAL
1	A	460	ARG
1	A	469	LEU
1	A	498	LEU
1	A	506	ILE
1	A	510	ARG
1	A	533	GLN
1	A	534	LYS
1	A	541	ARG
1	A	547	LEU
1	A	581	LEU
1	A	582	LEU
1	A	601	ARG
1	A	622	SER
1	A	652	THR
1	A	656	THR
1	B	60	ASP
1	B	89	TYR
1	B	91	GLU
1	B	92	ILE
1	B	103	LEU
1	B	107	LEU
1	B	112	ARG
1	B	125	GLU

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Mol	Chain	Res	Type
1	B	164	LYS
1	B	221	VAL
1	B	247	VAL
1	B	304	LEU
1	B	319	LEU
1	B	334	ARG
1	B	336	LEU
1	B	365	VAL
1	B	385	VAL
1	B	387	LEU
1	B	408	LEU
1	B	421	VAL
1	B	435	VAL
1	B	460	ARG
1	B	469	LEU
1	B	498	LEU
1	B	506	ILE
1	B	510	ARG
1	B	533	GLN
1	B	534	LYS
1	B	541	ARG
1	B	547	LEU
1	B	581	LEU
1	B	582	LEU
1	B	601	ARG
1	B	621	PRO
1	B	652	THR
1	B	656	THR
1	C	91	GLU
1	C	92	ILE
1	C	103	LEU
1	C	107	LEU
1	C	112	ARG
1	C	121	LEU
1	C	125	GLU
1	C	164	LYS
1	C	221	VAL
1	C	247	VAL
1	C	304	LEU
1	C	314	ARG
1	C	317	ARG
1	C	319	LEU

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Mol	Chain	Res	Type
1	C	334	ARG
1	C	336	LEU
1	C	385	VAL
1	C	387	LEU
1	C	408	LEU
1	C	421	VAL
1	C	435	VAL
1	C	460	ARG
1	C	469	LEU
1	C	498	LEU
1	C	506	ILE
1	C	510	ARG
1	C	528	ILE
1	C	533	GLN
1	C	534	LYS
1	C	541	ARG
1	C	547	LEU
1	C	581	LEU
1	C	582	LEU
1	C	601	ARG
1	C	622	SER
1	C	652	THR
1	C	656	THR
1	D	60	ASP
1	D	89	TYR
1	D	91	GLU
1	D	92	ILE
1	D	103	LEU
1	D	107	LEU
1	D	112	ARG
1	D	121	LEU
1	D	125	GLU
1	D	164	LYS
1	D	221	VAL
1	D	247	VAL
1	D	304	LEU
1	D	314	ARG
1	D	319	LEU
1	D	334	ARG
1	D	336	LEU
1	D	385	VAL
1	D	387	LEU

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Mol	Chain	Res	Type
1	D	408	LEU
1	D	421	VAL
1	D	435	VAL
1	D	460	ARG
1	D	469	LEU
1	D	498	LEU
1	D	506	ILE
1	D	510	ARG
1	D	533	GLN
1	D	534	LYS
1	D	547	LEU
1	D	581	LEU
1	D	582	LEU
1	D	601	ARG
1	D	652	THR
1	D	656	THR
1	E	91	GLU
1	E	92	ILE
1	E	103	LEU
1	E	107	LEU
1	E	112	ARG
1	E	121	LEU
1	E	125	GLU
1	E	164	LYS
1	E	221	VAL
1	E	247	VAL
1	E	304	LEU
1	E	314	ARG
1	E	317	ARG
1	E	319	LEU
1	E	336	LEU
1	E	385	VAL
1	E	387	LEU
1	E	408	LEU
1	E	421	VAL
1	E	435	VAL
1	E	460	ARG
1	E	469	LEU
1	E	498	LEU
1	E	506	ILE
1	E	533	GLN
1	E	534	LYS

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Mol	Chain	Res	Type
1	E	541	ARG
1	E	547	LEU
1	E	581	LEU
1	E	582	LEU
1	E	601	ARG
1	E	621	PRO
1	E	622	SER
1	E	652	THR
1	E	656	THR
1	F	60	ASP
1	F	91	GLU
1	F	92	ILE
1	F	103	LEU
1	F	107	LEU
1	F	112	ARG
1	F	121	LEU
1	F	125	GLU
1	F	164	LYS
1	F	184	ASN
1	F	196	THR
1	F	221	VAL
1	F	247	VAL
1	F	304	LEU
1	F	317	ARG
1	F	319	LEU
1	F	336	LEU
1	F	385	VAL
1	F	387	LEU
1	F	408	LEU
1	F	421	VAL
1	F	435	VAL
1	F	460	ARG
1	F	469	LEU
1	F	498	LEU
1	F	506	ILE
1	F	510	ARG
1	F	533	GLN
1	F	534	LYS
1	F	541	ARG
1	F	547	LEU
1	F	581	LEU
1	F	582	LEU

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Mol	Chain	Res	Type
1	F	601	ARG
1	F	621	PRO
1	F	622	SER
1	F	652	THR
1	F	656	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (137) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	HIS
1	A	102	ASN
1	A	147	GLN
1	A	175	GLN
1	A	190	GLN
1	A	238	GLN
1	A	248	HIS
1	A	288	GLN
1	A	324	ASN
1	A	329	ASN
1	A	363	HIS
1	A	372	HIS
1	A	379	HIS
1	A	401	ASN
1	A	448	HIS
1	A	502	ASN
1	A	514	GLN
1	A	518	ASN
1	A	533	GLN
1	A	564	ASN
1	A	567	ASN
1	A	588	HIS
1	A	639	GLN
1	B	64	HIS
1	B	102	ASN
1	B	175	GLN
1	B	190	GLN
1	B	218	HIS
1	B	248	HIS
1	B	288	GLN
1	B	324	ASN
1	B	329	ASN
1	B	363	HIS

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Mol	Chain	Res	Type
1	B	372	HIS
1	B	379	HIS
1	B	401	ASN
1	B	502	ASN
1	B	514	GLN
1	B	518	ASN
1	B	533	GLN
1	B	564	ASN
1	B	567	ASN
1	B	588	HIS
1	B	639	GLN
1	C	64	HIS
1	C	102	ASN
1	C	118	ASN
1	C	133	HIS
1	C	147	GLN
1	C	171	GLN
1	C	175	GLN
1	C	190	GLN
1	C	238	GLN
1	C	248	HIS
1	C	288	GLN
1	C	324	ASN
1	C	329	ASN
1	C	363	HIS
1	C	372	HIS
1	C	379	HIS
1	C	401	ASN
1	C	448	HIS
1	C	502	ASN
1	C	514	GLN
1	C	518	ASN
1	C	533	GLN
1	C	564	ASN
1	C	567	ASN
1	C	588	HIS
1	C	639	GLN
1	D	102	ASN
1	D	147	GLN
1	D	175	GLN
1	D	190	GLN
1	D	218	HIS

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Mol	Chain	Res	Type
1	D	288	GLN
1	D	324	ASN
1	D	329	ASN
1	D	363	HIS
1	D	372	HIS
1	D	379	HIS
1	D	401	ASN
1	D	514	GLN
1	D	518	ASN
1	D	533	GLN
1	D	564	ASN
1	D	567	ASN
1	D	588	HIS
1	D	639	GLN
1	E	118	ASN
1	E	133	HIS
1	E	147	GLN
1	E	175	GLN
1	E	190	GLN
1	E	218	HIS
1	E	238	GLN
1	E	248	HIS
1	E	288	GLN
1	E	324	ASN
1	E	329	ASN
1	E	363	HIS
1	E	372	HIS
1	E	379	HIS
1	E	401	ASN
1	E	502	ASN
1	E	514	GLN
1	E	518	ASN
1	E	533	GLN
1	E	564	ASN
1	E	567	ASN
1	E	588	HIS
1	E	639	GLN
1	F	64	HIS
1	F	102	ASN
1	F	118	ASN
1	F	147	GLN
1	F	175	GLN

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Mol	Chain	Res	Type
1	F	190	GLN
1	F	218	HIS
1	F	238	GLN
1	F	248	HIS
1	F	288	GLN
1	F	324	ASN
1	F	329	ASN
1	F	363	HIS
1	F	372	HIS
1	F	379	HIS
1	F	401	ASN
1	F	502	ASN
1	F	514	GLN
1	F	518	ASN
1	F	533	GLN
1	F	564	ASN
1	F	567	ASN
1	F	588	HIS
1	F	592	HIS
1	F	639	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	UGA	A	1101	-	38,39,39	0.89	2 (5%)	56,60,60	0.95	3 (5%)
2	ATP	C	1003	-	32,33,33	0.90	2 (6%)	48,52,52	0.98	3 (6%)
3	UGA	E	1105	-	38,39,39	0.88	3 (7%)	56,60,60	0.97	2 (3%)
2	ATP	D	1004	-	32,33,33	1.08	3 (9%)	48,52,52	0.98	2 (4%)
3	UGA	F	1106	-	38,39,39	0.97	3 (7%)	56,60,60	0.99	2 (3%)
3	UGA	C	1103	-	38,39,39	0.85	2 (5%)	56,60,60	0.98	2 (3%)
2	ATP	E	1005	-	32,33,33	0.74	1 (3%)	48,52,52	0.99	2 (4%)
3	UGA	B	1102	-	38,39,39	0.91	3 (7%)	56,60,60	1.00	3 (5%)
2	ATP	F	1006	-	32,33,33	0.97	2 (6%)	48,52,52	0.99	3 (6%)
2	ATP	A	1001	-	32,33,33	0.84	1 (3%)	48,52,52	1.03	2 (4%)
3	UGA	D	1104	-	38,39,39	0.87	2 (5%)	56,60,60	0.93	3 (5%)
2	ATP	B	1002	-	32,33,33	0.83	1 (3%)	48,52,52	0.99	2 (4%)

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
3	UGA	A	1101	-	-	4/25/61/61	0/3/3/3
2	ATP	C	1003	-	-	4/22/38/38	0/3/3/3
3	UGA	E	1105	-	-	4/25/61/61	0/3/3/3
2	ATP	D	1004	-	-	4/22/38/38	0/3/3/3
3	UGA	F	1106	-	-	4/25/61/61	0/3/3/3
3	UGA	C	1103	-	-	4/25/61/61	0/3/3/3
2	ATP	E	1005	-	-	4/22/38/38	0/3/3/3
3	UGA	B	1102	-	-	4/25/61/61	0/3/3/3
2	ATP	F	1006	-	-	4/22/38/38	0/3/3/3
2	ATP	A	1001	-	-	4/22/38/38	0/3/3/3
3	UGA	D	1104	-	-	4/25/61/61	0/3/3/3
2	ATP	B	1002	-	-	4/22/38/38	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1006	ATP	PB-O3B	3.91	1.63	1.59
2	D	1004	ATP	PB-O3B	3.84	1.63	1.59
2	C	1003	ATP	PB-O3B	3.65	1.63	1.59
2	A	1001	ATP	PB-O3B	3.43	1.63	1.59
2	B	1002	ATP	PB-O3B	3.37	1.63	1.59
2	D	1004	ATP	PB-O3A	3.28	1.63	1.59
3	F	1106	UGA	PA-O3A	3.22	1.63	1.59
2	E	1005	ATP	PB-O3B	3.13	1.62	1.59
3	B	1102	UGA	PA-O3A	3.00	1.62	1.59
3	D	1104	UGA	PA-O3A	2.80	1.62	1.59
3	A	1101	UGA	PA-O3A	2.79	1.62	1.59
3	E	1105	UGA	PA-O3A	2.78	1.62	1.59
3	F	1106	UGA	PB-O3A	2.51	1.62	1.59
2	D	1004	ATP	PA-O3A	2.51	1.62	1.59
3	C	1103	UGA	PA-O3A	2.48	1.62	1.59
3	A	1101	UGA	O'P-C6'	2.45	1.29	1.22
3	F	1106	UGA	O'P-C6'	2.45	1.29	1.22
3	C	1103	UGA	O'P-C6'	2.38	1.29	1.22
3	B	1102	UGA	PB-O3A	2.38	1.62	1.59
3	D	1104	UGA	O'P-C6'	2.30	1.28	1.22
2	F	1006	ATP	PB-O3A	2.20	1.61	1.59
3	B	1102	UGA	O'P-C6'	2.16	1.28	1.22
3	E	1105	UGA	PB-O3A	2.14	1.61	1.59
2	C	1003	ATP	PB-O3A	2.10	1.61	1.59
3	E	1105	UGA	O'P-C6'	2.10	1.28	1.22

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1102	UGA	O5'-C1'-O3B	4.86	117.71	111.36
3	F	1106	UGA	O5'-C1'-O3B	4.83	117.68	111.36
3	A	1101	UGA	O5'-C1'-O3B	4.80	117.64	111.36
3	D	1104	UGA	O5'-C1'-O3B	4.61	117.39	111.36
3	C	1103	UGA	O5'-C1'-O3B	4.60	117.38	111.36
3	E	1105	UGA	O5'-C1'-O3B	4.54	117.30	111.36
3	B	1102	UGA	O2B-PB-O3A	-3.02	99.12	107.27
3	C	1103	UGA	O2B-PB-O3A	-2.98	99.22	107.27
3	F	1106	UGA	O2B-PB-O3A	-2.59	100.28	107.27
2	A	1001	ATP	O4'-C1'-N9	2.57	113.02	108.09
3	E	1105	UGA	O2B-PB-O3A	-2.54	100.41	107.27
2	D	1004	ATP	O4'-C1'-N9	2.50	112.89	108.09
3	A	1101	UGA	O2B-PB-O3A	-2.46	100.62	107.27
2	C	1003	ATP	O4'-C1'-N9	2.30	112.50	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1005	ATP	O4'-C1'-N9	2.30	112.50	108.09
2	B	1002	ATP	O4'-C1'-N9	2.28	112.46	108.09
3	D	1104	UGA	O2B-PB-O3A	-2.21	101.30	107.27
2	B	1002	ATP	O3G-PG-O2G	2.15	115.87	107.80
2	F	1006	ATP	O4'-C1'-N9	2.14	112.20	108.09
2	A	1001	ATP	O3G-PG-O2G	2.13	115.78	107.80
2	D	1004	ATP	O3G-PG-O2G	2.11	115.72	107.80
3	B	1102	UGA	C1'-O5'-C5'	2.11	115.69	112.23
2	C	1003	ATP	O3G-PG-O2G	2.10	115.67	107.80
2	F	1006	ATP	O3G-PG-O2G	2.09	115.66	107.80
2	C	1003	ATP	C1'-N9-C8	2.07	131.70	127.09
2	E	1005	ATP	O3G-PG-O2G	2.07	115.57	107.80
2	F	1006	ATP	C2'-C1'-N9	2.06	118.42	113.30
3	D	1104	UGA	C1'-O5'-C5'	2.04	115.57	112.23
3	A	1101	UGA	C1'-O5'-C5'	2.03	115.56	112.23

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ATP	C5'-O5'-PA-O2A
2	A	1001	ATP	C5'-O5'-PA-O3A
2	B	1002	ATP	C5'-O5'-PA-O2A
2	C	1003	ATP	C5'-O5'-PA-O2A
2	D	1004	ATP	C5'-O5'-PA-O2A
2	E	1005	ATP	C5'-O5'-PA-O2A
2	E	1005	ATP	C5'-O5'-PA-O3A
2	F	1006	ATP	C5'-O5'-PA-O2A
2	F	1006	ATP	C5'-O5'-PA-O3A
3	B	1102	UGA	C5D-O5D-PA-O3A
3	C	1103	UGA	C5D-O5D-PA-O3A
3	D	1104	UGA	C5D-O5D-PA-O3A
3	E	1105	UGA	C5D-O5D-PA-O3A
3	A	1101	UGA	C2'-C1'-O3B-PB
3	B	1102	UGA	C2'-C1'-O3B-PB
3	C	1103	UGA	C2'-C1'-O3B-PB
3	D	1104	UGA	C2'-C1'-O3B-PB
3	E	1105	UGA	C2'-C1'-O3B-PB
3	F	1106	UGA	C2'-C1'-O3B-PB
3	A	1101	UGA	PB-O3A-PA-O1A
3	B	1102	UGA	PB-O3A-PA-O1A
3	C	1103	UGA	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	D	1104	UGA	PB-O3A-PA-O1A
3	E	1105	UGA	PB-O3A-PA-O1A
3	F	1106	UGA	PB-O3A-PA-O1A
2	A	1001	ATP	C5'-O5'-PA-O1A
2	B	1002	ATP	C5'-O5'-PA-O1A
2	B	1002	ATP	C5'-O5'-PA-O3A
2	C	1003	ATP	C5'-O5'-PA-O1A
2	C	1003	ATP	C5'-O5'-PA-O3A
2	D	1004	ATP	C5'-O5'-PA-O1A
2	D	1004	ATP	C5'-O5'-PA-O3A
2	E	1005	ATP	C5'-O5'-PA-O1A
2	F	1006	ATP	C5'-O5'-PA-O1A
3	A	1101	UGA	C5D-O5D-PA-O3A
3	F	1106	UGA	C5D-O5D-PA-O3A
3	A	1101	UGA	PB-O3A-PA-O2A
3	B	1102	UGA	PB-O3A-PA-O2A
3	E	1105	UGA	PB-O3A-PA-O2A
3	F	1106	UGA	PB-O3A-PA-O2A
2	B	1002	ATP	C4'-C5'-O5'-PA
2	E	1005	ATP	C4'-C5'-O5'-PA
2	F	1006	ATP	C4'-C5'-O5'-PA
3	C	1103	UGA	PB-O3A-PA-O2A
3	D	1104	UGA	PB-O3A-PA-O2A
2	A	1001	ATP	C4'-C5'-O5'-PA
2	C	1003	ATP	C4'-C5'-O5'-PA
2	D	1004	ATP	C4'-C5'-O5'-PA

There are no ring outliers.

12 monomers are involved in 28 short contacts:

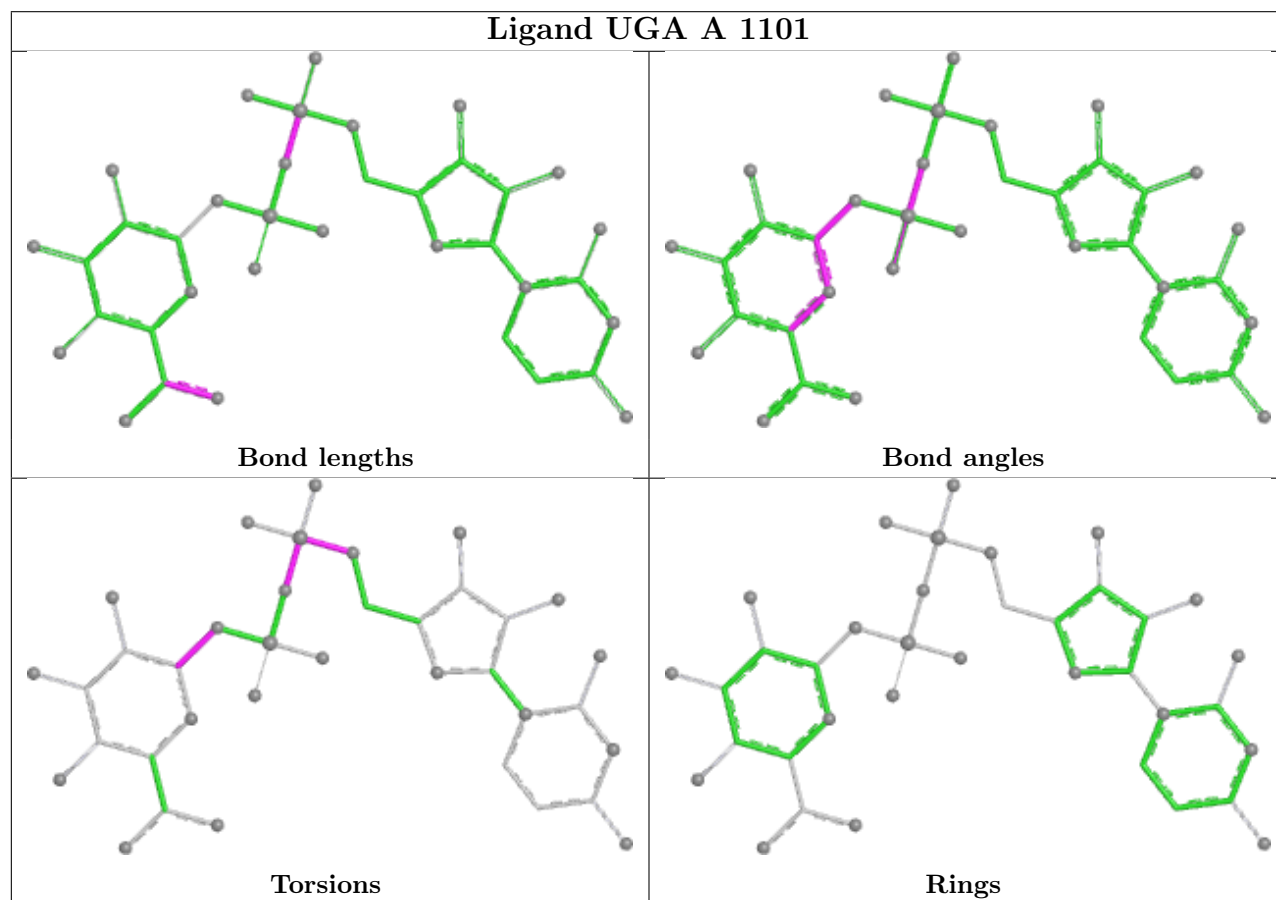
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1101	UGA	1	0
2	C	1003	ATP	4	0
3	E	1105	UGA	1	0
2	D	1004	ATP	4	0
3	F	1106	UGA	1	0
3	C	1103	UGA	1	0
2	E	1005	ATP	2	0
3	B	1102	UGA	1	0
2	F	1006	ATP	3	0
2	A	1001	ATP	5	0
3	D	1104	UGA	1	0

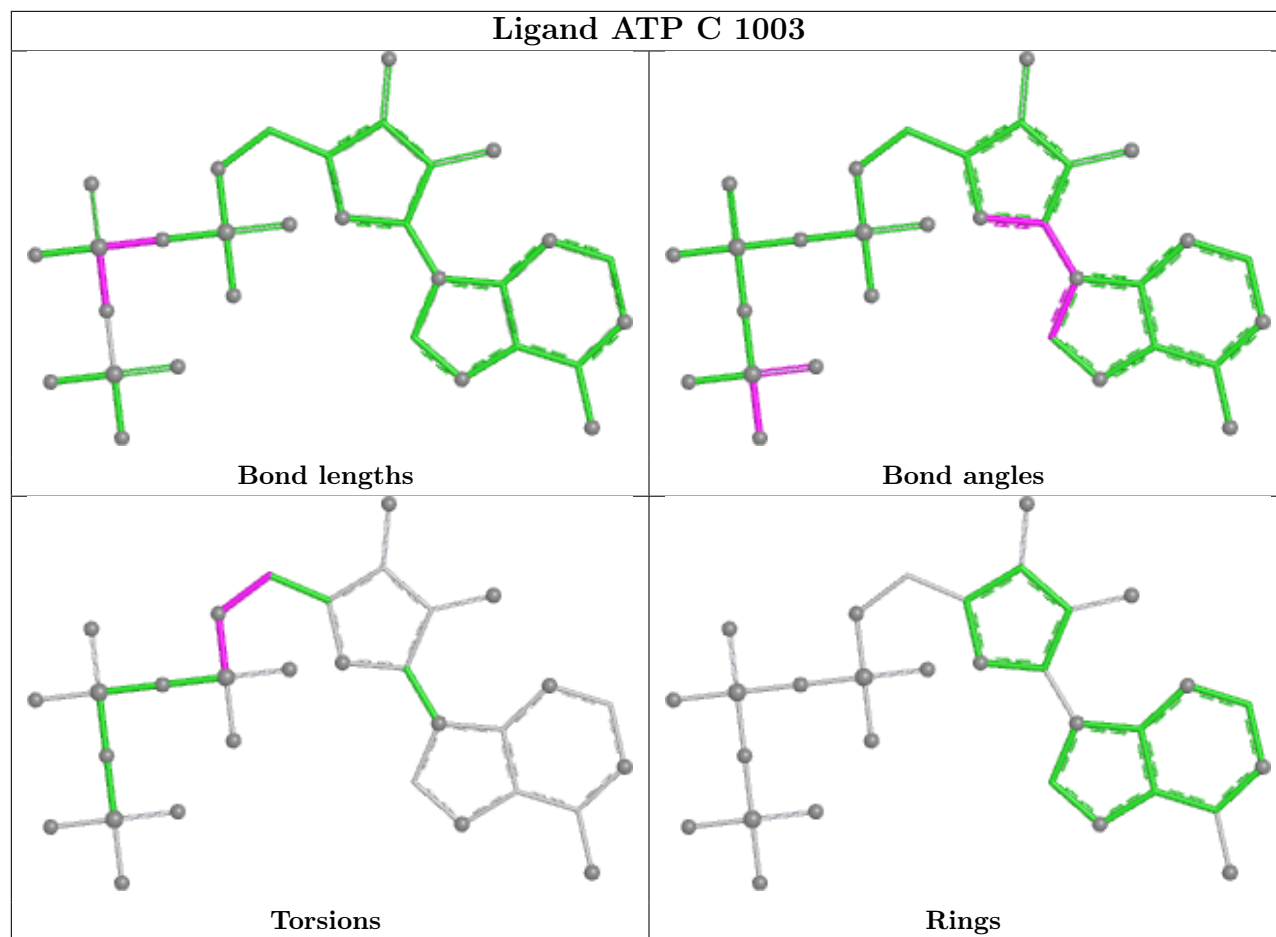
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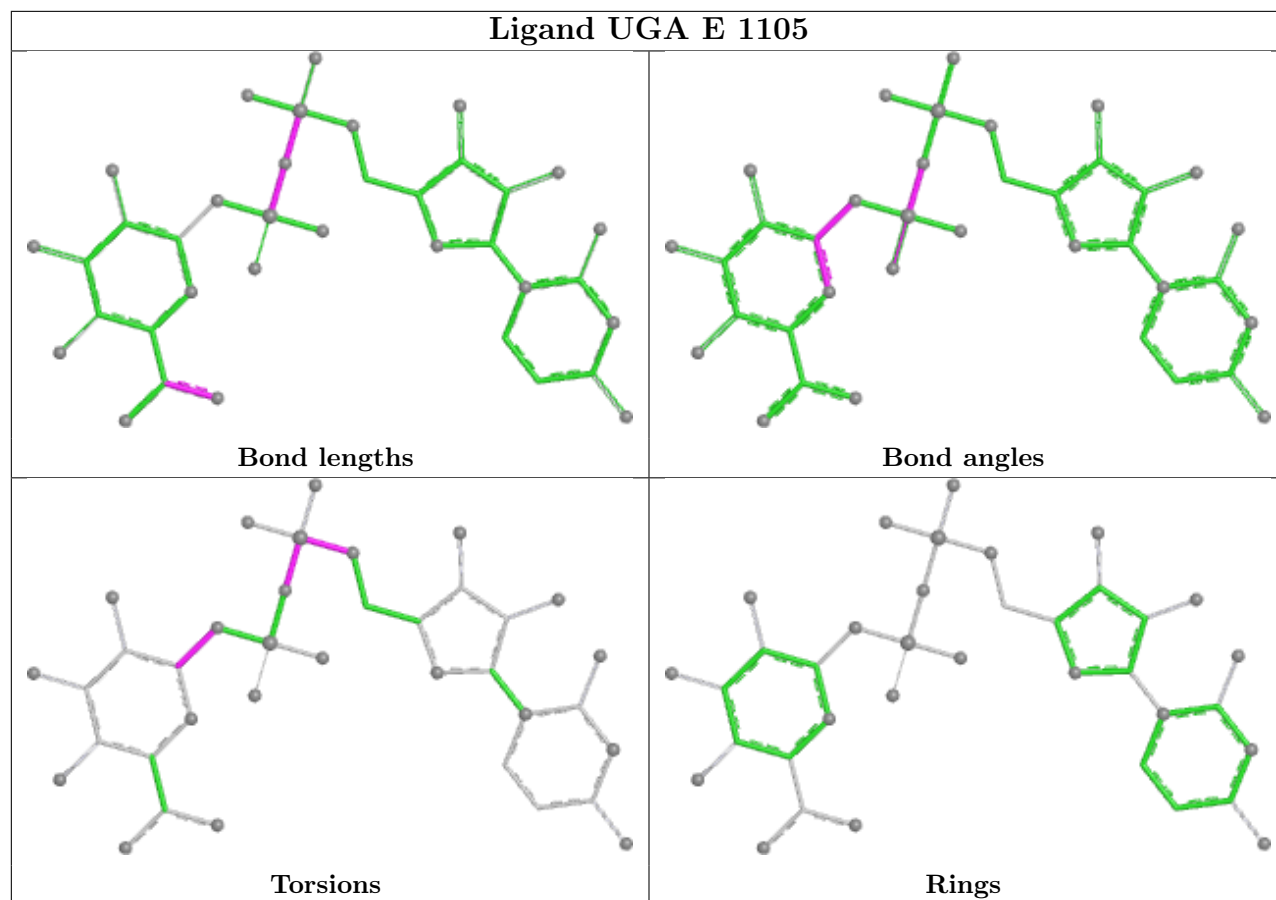
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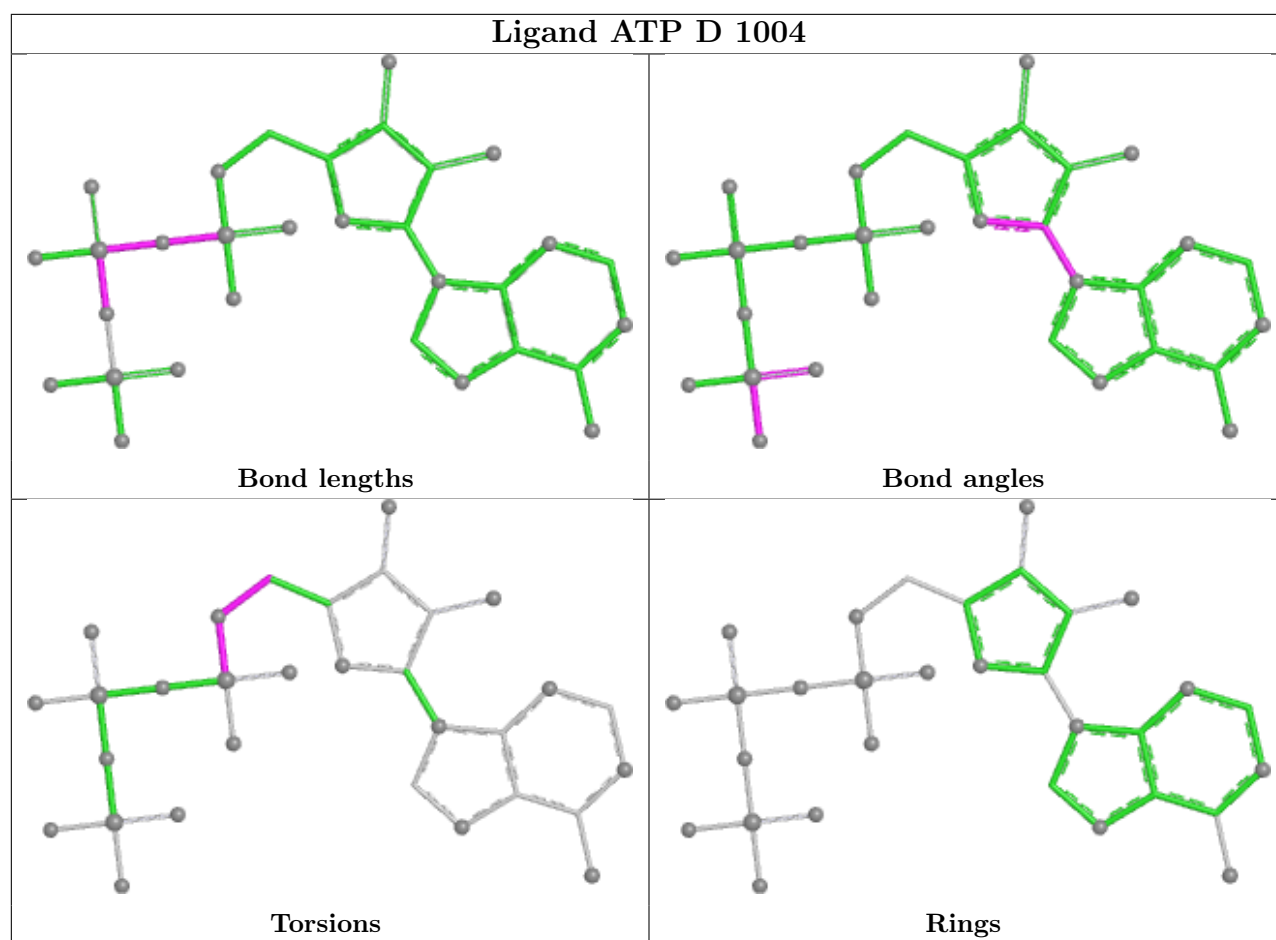
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1002	ATP	4	0

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.

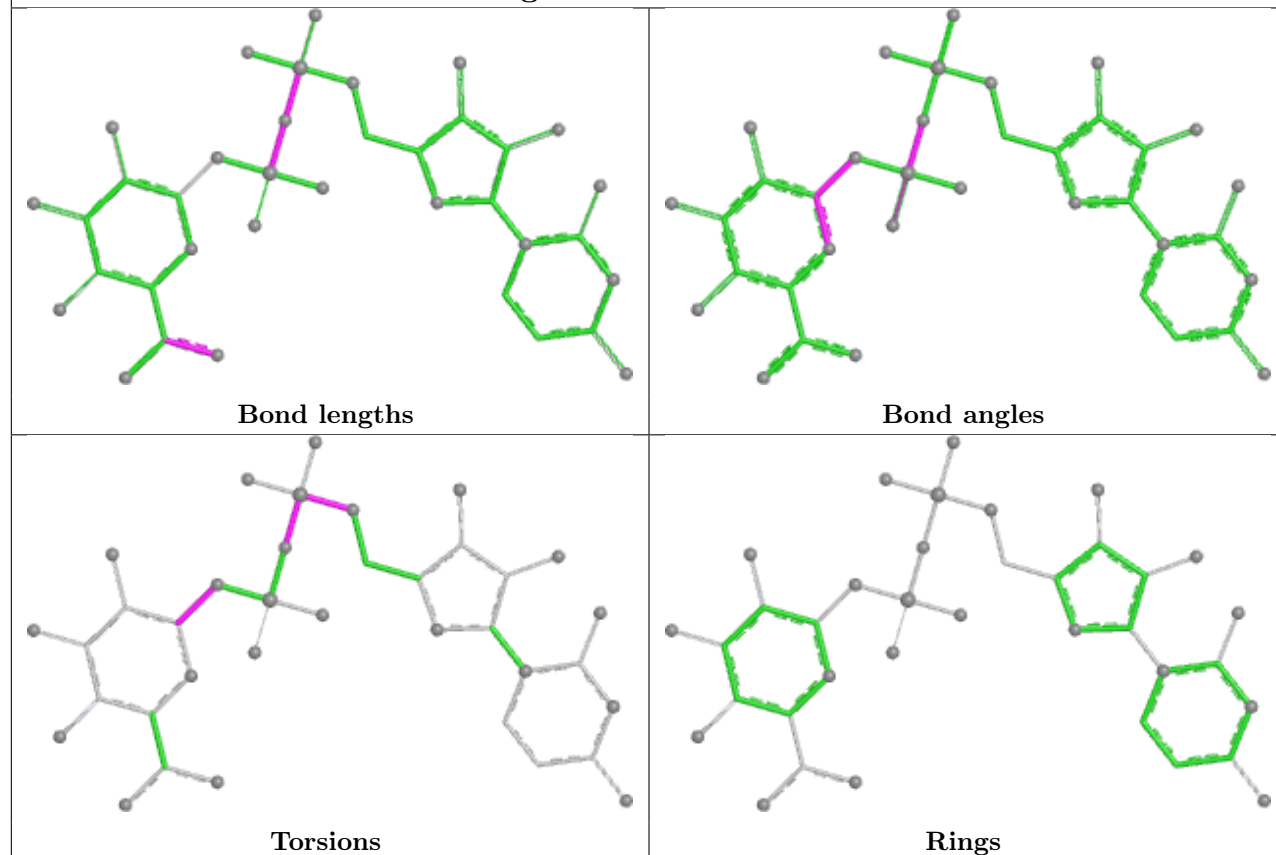




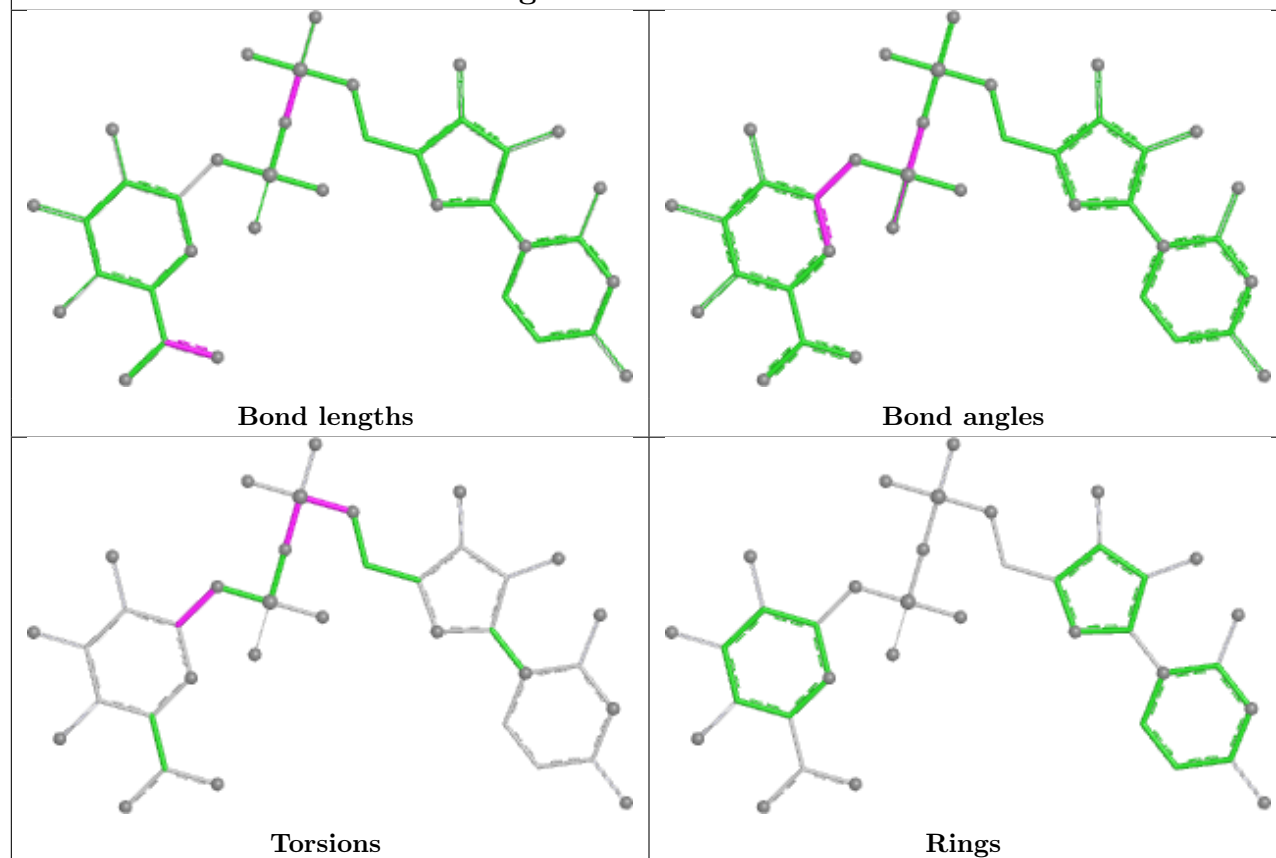


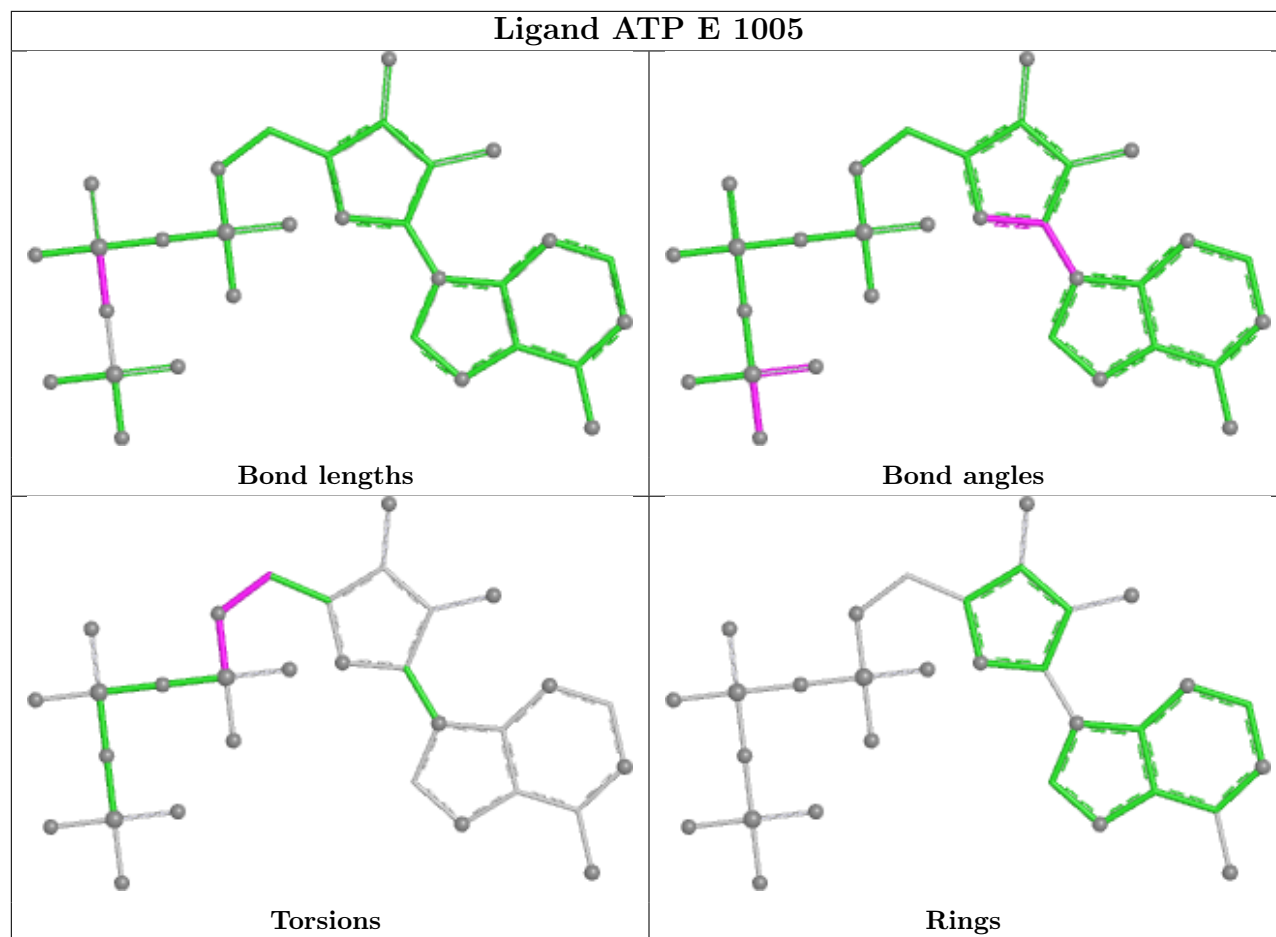


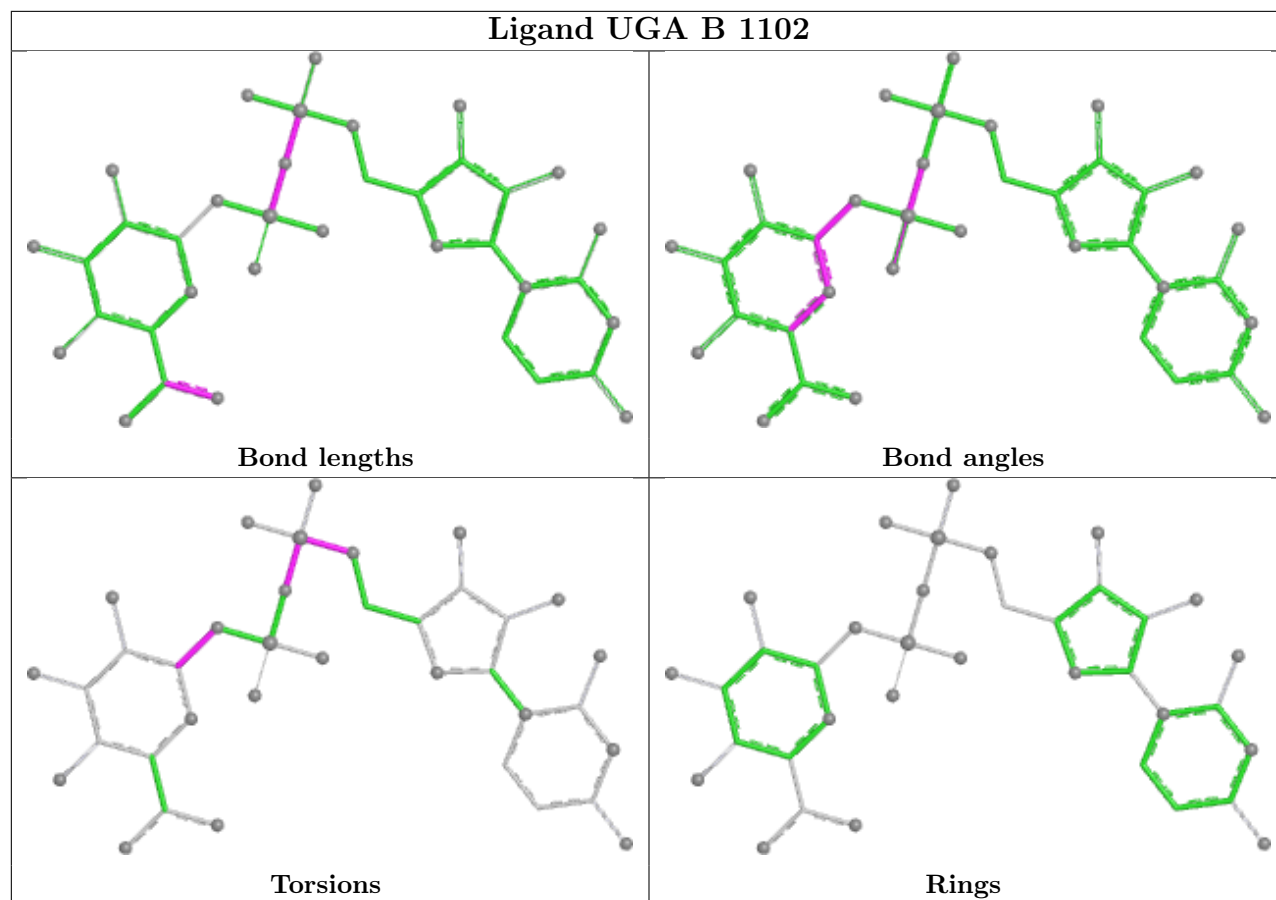
Ligand UGA F 1106

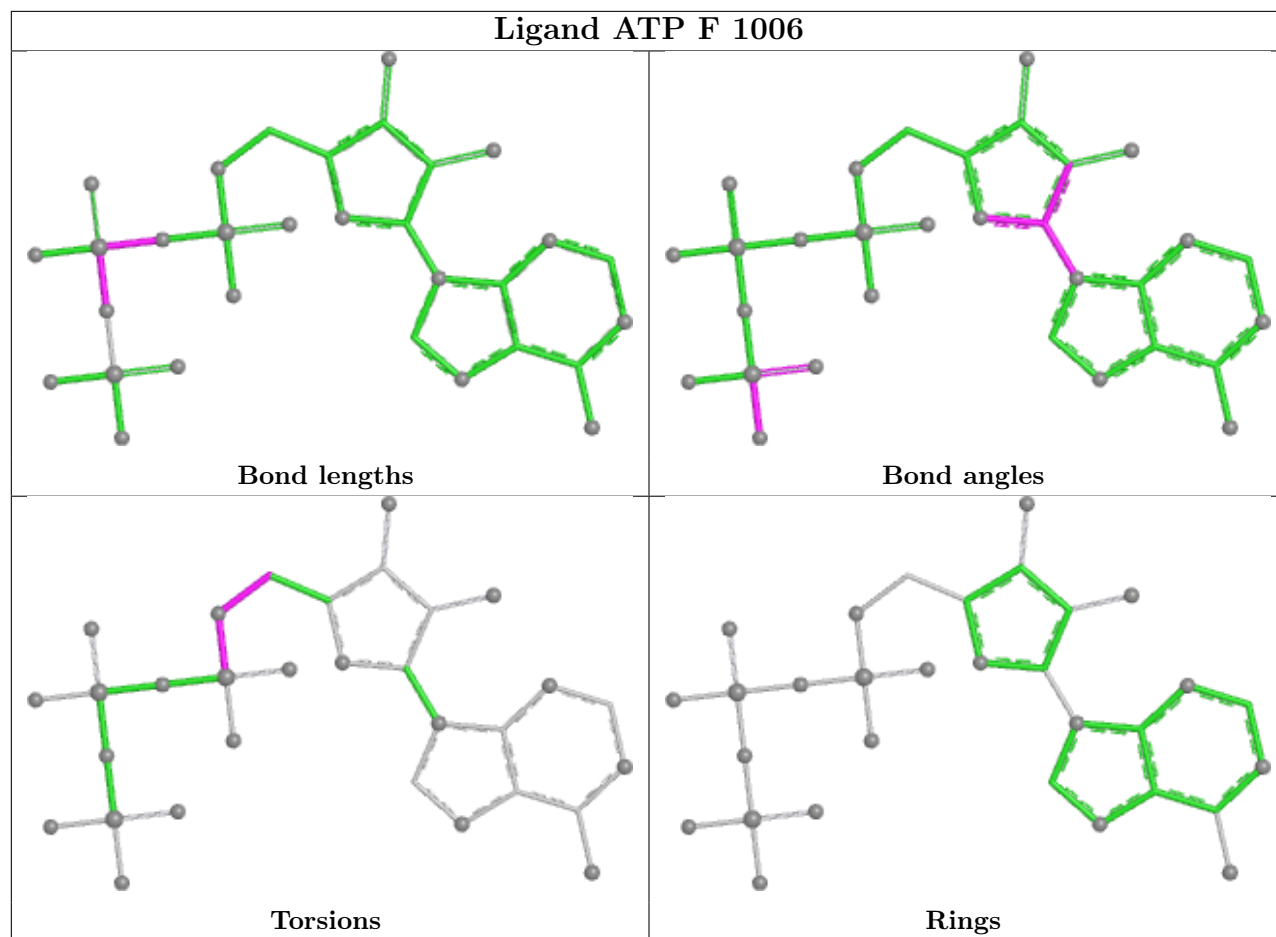


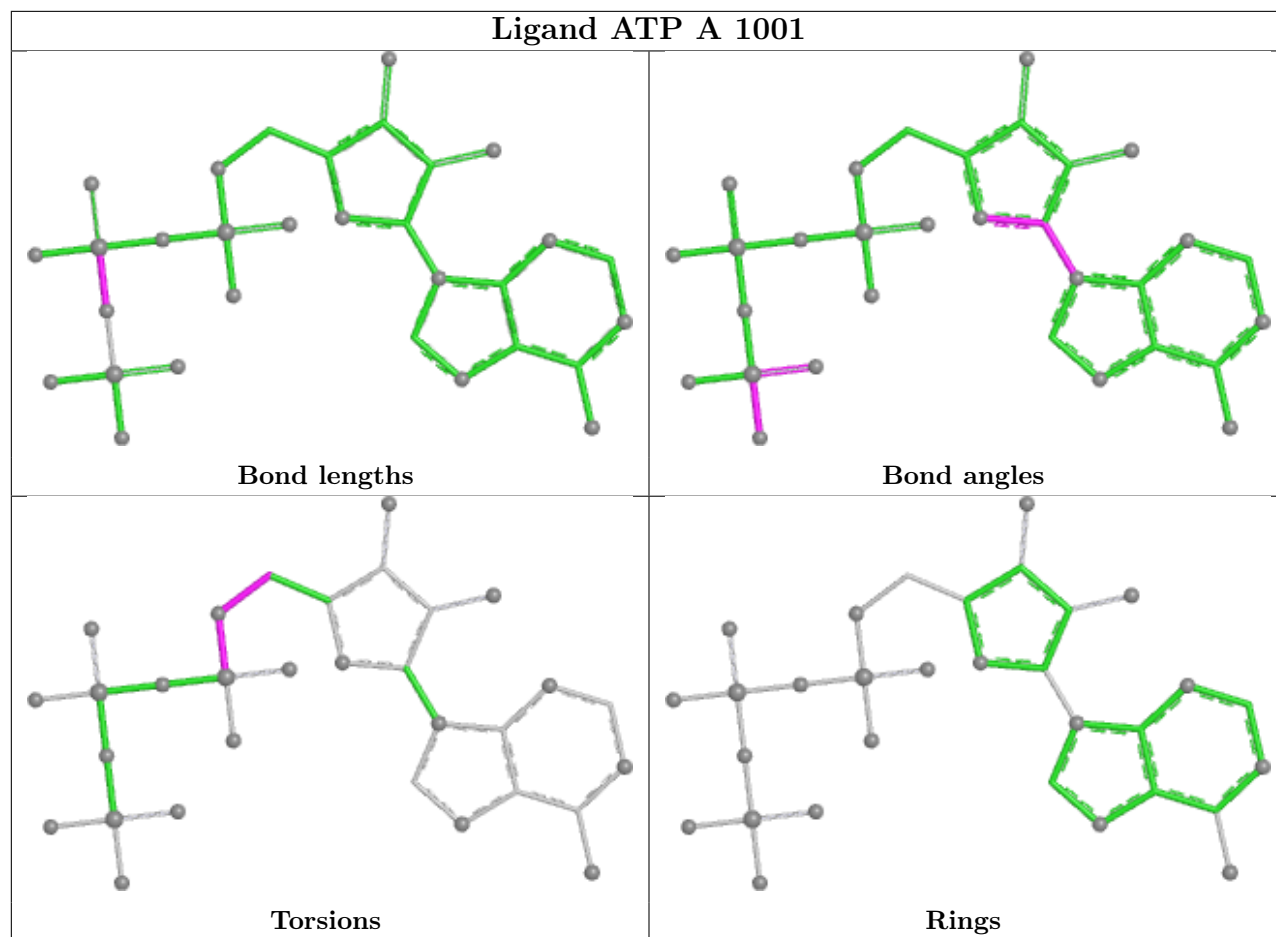
Ligand UGA C 1103



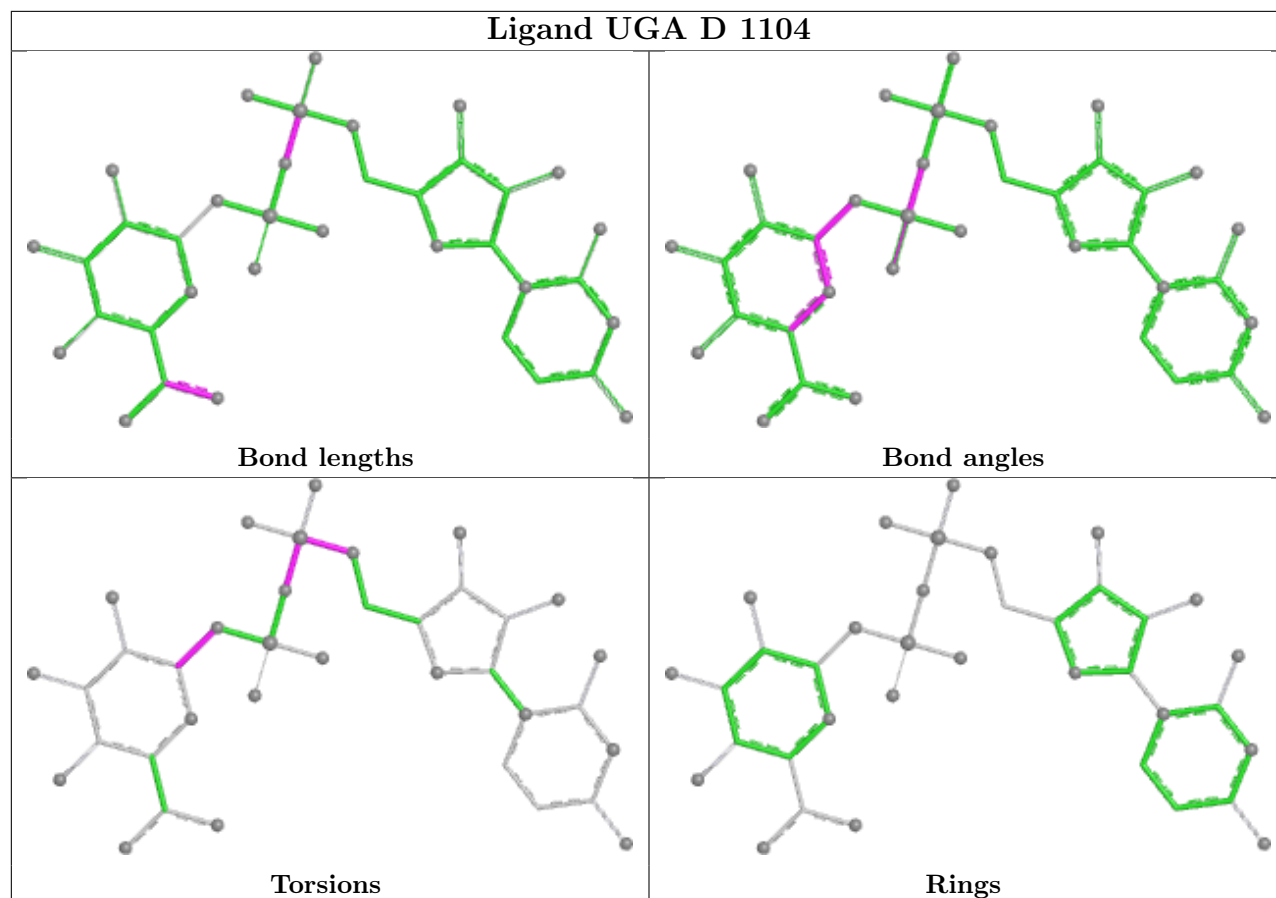


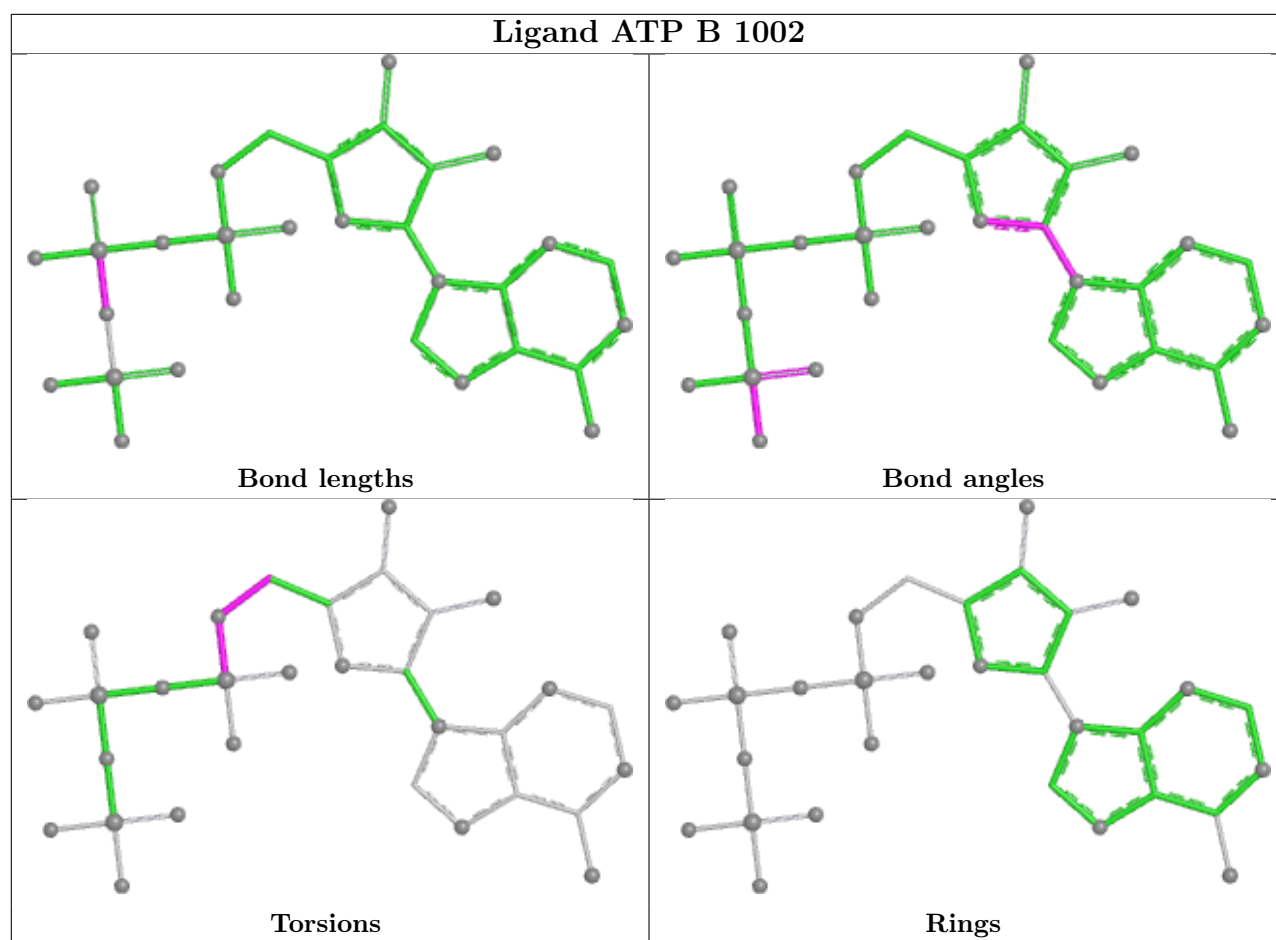






Ligand UGA D 1104





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	639/660 (96%)	0.23	32 (5%)	34	18	20, 43, 74, 90	0
1	B	639/660 (96%)	0.27	43 (6%)	24	12	19, 43, 73, 90	0
1	C	639/660 (96%)	0.33	39 (6%)	27	14	20, 43, 73, 90	0
1	D	644/660 (97%)	0.22	37 (5%)	29	15	20, 44, 74, 90	0
1	E	639/660 (96%)	0.16	25 (3%)	43	24	20, 44, 73, 90	0
1	F	639/660 (96%)	0.51	91 (14%)	6	4	19, 43, 75, 91	0
All	All	3839/3960 (96%)	0.29	267 (6%)	22	12	19, 43, 74, 91	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	656	THR	6.7
1	B	184	ASN	5.8
1	C	187	GLU	5.7
1	E	253	LYS	5.4
1	D	656	THR	5.3
1	F	250	HIS	5.1
1	A	656	THR	5.0
1	C	655	LEU	4.9
1	F	22	ALA	4.8
1	A	186	LEU	4.7
1	A	171	GLN	4.6
1	A	175	GLN	4.6
1	D	308	PRO	4.6
1	B	187	GLU	4.4
1	B	188	ILE	4.3
1	F	252	SER	4.2
1	B	302	SER	4.2
1	F	251	ALA	4.2
1	B	235	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	E	302	SER	4.1
1	A	187	GLU	4.1
1	B	186	LEU	4.1
1	D	655	LEU	4.1
1	D	251	ALA	4.1
1	D	186	LEU	3.9
1	F	189	ALA	3.9
1	F	186	LEU	3.9
1	C	87	LEU	3.9
1	A	250	HIS	3.8
1	B	237	ASN	3.8
1	C	186	LEU	3.7
1	B	252	SER	3.7
1	E	656	THR	3.7
1	F	1	MET	3.6
1	F	656	THR	3.6
1	F	188	ILE	3.6
1	B	253	LYS	3.6
1	C	86	HIS	3.6
1	D	302	SER	3.6
1	C	90	ASP	3.6
1	C	167	HIS	3.6
1	C	251	ALA	3.5
1	A	185	ILE	3.5
1	F	91	GLU	3.5
1	D	43	GLY	3.5
1	F	253	LYS	3.5
1	F	187	GLU	3.5
1	A	188	ILE	3.4
1	F	101	PHE	3.4
1	F	90	ASP	3.4
1	F	177	LEU	3.4
1	A	184	ASN	3.4
1	B	251	ALA	3.4
1	E	251	ALA	3.3
1	D	86	HIS	3.3
1	C	185	ILE	3.3
1	E	252	SER	3.3
1	B	182	HIS	3.3
1	D	307	GLN	3.3
1	E	87	LEU	3.3
1	A	251	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	43	GLY	3.2
1	F	137	LYS	3.2
1	E	250	HIS	3.2
1	B	183	GLY	3.2
1	C	615	ASP	3.2
1	C	250	HIS	3.2
1	F	105	GLY	3.1
1	F	183	GLY	3.1
1	B	250	HIS	3.1
1	E	90	ASP	3.1
1	C	91	GLU	3.1
1	E	187	GLU	3.1
1	C	92	ILE	3.1
1	D	252	SER	3.1
1	F	98	ALA	3.1
1	E	186	LEU	3.1
1	E	43	GLY	3.1
1	C	188	ILE	3.1
1	D	87	LEU	3.0
1	F	146	ALA	3.0
1	F	302	SER	3.0
1	C	89	TYR	3.0
1	F	86	HIS	3.0
1	B	304	LEU	2.9
1	B	254	ALA	2.9
1	F	99	GLY	2.9
1	C	189	ALA	2.9
1	F	93	LEU	2.9
1	B	656	THR	2.9
1	B	90	ASP	2.9
1	A	183	GLY	2.9
1	F	185	ILE	2.9
1	F	141	ALA	2.8
1	D	89	TYR	2.8
1	D	187	GLU	2.8
1	B	179	ALA	2.8
1	B	255	GLN	2.8
1	C	271	ASP	2.8
1	B	87	LEU	2.8
1	C	654	ASP	2.7
1	E	301	GLY	2.7
1	F	23	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	2.7
1	F	127	GLU	2.7
1	A	253	LYS	2.7
1	C	653	VAL	2.7
1	A	87	LEU	2.7
1	F	304	LEU	2.7
1	F	184	ASN	2.7
1	F	21	ALA	2.7
1	A	89	TYR	2.7
1	F	111	TYR	2.7
1	E	304	LEU	2.6
1	C	249	PRO	2.6
1	F	178	PRO	2.6
1	C	34	ASP	2.6
1	C	237	ASN	2.6
1	C	43	GLY	2.6
1	E	182	HIS	2.6
1	F	24	TYR	2.6
1	B	203	PRO	2.6
1	A	204	ASP	2.6
1	A	615	ASP	2.6
1	A	43	GLY	2.6
1	E	188	ILE	2.6
1	A	90	ASP	2.6
1	E	631	ASP	2.6
1	F	204	ASP	2.6
1	C	191	ARG	2.6
1	F	203	PRO	2.5
1	B	301	GLY	2.5
1	F	108	LEU	2.5
1	E	303	ARG	2.5
1	B	249	PRO	2.5
1	F	182	HIS	2.5
1	B	94	GLN	2.5
1	C	183	GLY	2.5
1	F	121	LEU	2.5
1	F	27	SER	2.5
1	B	193	ASN	2.5
1	F	150	ILE	2.5
1	B	592	HIS	2.5
1	F	249	PRO	2.5
1	F	62	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	95	LEU	2.5
1	F	256	PRO	2.5
1	D	193	ASN	2.4
1	F	76	PRO	2.4
1	B	89	TYR	2.4
1	D	182	HIS	2.4
1	F	190	GLN	2.4
1	F	148	LEU	2.4
1	A	176	THR	2.4
1	B	615	ASP	2.4
1	F	77	ASP	2.4
1	D	249	PRO	2.4
1	F	97	PRO	2.4
1	B	66	LEU	2.4
1	F	131	THR	2.4
1	F	196	THR	2.4
1	A	86	HIS	2.4
1	F	89	TYR	2.4
1	F	92	ILE	2.4
1	F	135	MET	2.4
1	F	132	LEU	2.4
1	F	176	THR	2.4
1	B	631	ASP	2.4
1	D	1	MET	2.4
1	E	300	GLN	2.4
1	A	203	PRO	2.4
1	F	180	ILE	2.3
1	D	34	ASP	2.3
1	D	654	ASP	2.3
1	D	200	ARG	2.3
1	F	134	ARG	2.3
1	F	195	ALA	2.3
1	A	182	HIS	2.3
1	F	211	HIS	2.3
1	A	655	LEU	2.3
1	F	63	ASN	2.3
1	B	204	ASP	2.3
1	F	68	VAL	2.3
1	C	85	ARG	2.3
1	B	150	ILE	2.3
1	B	185	ILE	2.3
1	D	188	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	2.2
1	F	139	ALA	2.2
1	F	181	LYS	2.2
1	D	303	ARG	2.2
1	A	34	ASP	2.2
1	F	174	GLU	2.2
1	F	71	ILE	2.2
1	C	196	THR	2.2
1	F	167	HIS	2.2
1	B	73	GLN	2.2
1	E	146	ALA	2.2
1	D	253	LYS	2.2
1	C	200	ARG	2.2
1	F	237	ASN	2.2
1	C	304	LEU	2.2
1	B	189	ALA	2.2
1	C	257	GLY	2.2
1	F	65	PRO	2.2
1	F	113	GLY	2.2
1	D	204	ASP	2.2
1	B	138	ARG	2.2
1	D	255	GLN	2.2
1	A	237	ASN	2.2
1	F	25	GLU	2.2
1	D	615	ASP	2.2
1	D	9	HIS	2.2
1	F	64	HIS	2.2
1	F	87	LEU	2.1
1	C	146	ALA	2.1
1	A	85	ARG	2.1
1	D	91	GLU	2.1
1	B	207	PHE	2.1
1	B	34	ASP	2.1
1	E	34	ASP	2.1
1	F	615	ASP	2.1
1	C	235	VAL	2.1
1	D	235	VAL	2.1
1	F	67	TRP	2.1
1	D	185	ILE	2.1
1	B	655	LEU	2.1
1	F	200	ARG	2.1
1	F	193	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	62	VAL	2.1
1	B	86	HIS	2.1
1	E	655	LEU	2.1
1	F	88	ILE	2.1
1	A	114	ARG	2.1
1	C	149	ARG	2.1
1	F	209	GLU	2.1
1	A	252	SER	2.1
1	F	80	PHE	2.1
1	E	204	ASP	2.1
1	F	248	HIS	2.1
1	A	238	GLN	2.1
1	C	190	GLN	2.1
1	D	300	GLN	2.1
1	A	249	PRO	2.1
1	E	193	ASN	2.1
1	C	88	ILE	2.1
1	D	85	ARG	2.1
1	F	303	ARG	2.1
1	F	34	ASP	2.1
1	F	631	ASP	2.1
1	D	73	GLN	2.1
1	F	129	GLY	2.1
1	B	303	ARG	2.0
1	B	196	THR	2.0
1	D	195	ALA	2.0
1	F	202	THR	2.0
1	E	235	VAL	2.0
1	B	601	ARG	2.0
1	F	66	LEU	2.0
1	D	254	ALA	2.0
1	F	28	ALA	2.0
1	C	204	ASP	2.0
1	D	301	GLY	2.0
1	E	249	PRO	2.0
1	F	94	GLN	2.0
1	C	93	LEU	2.0
1	D	92	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

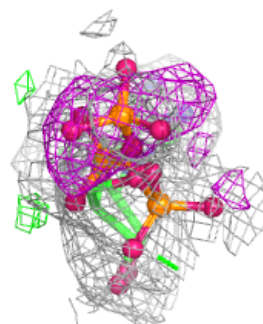
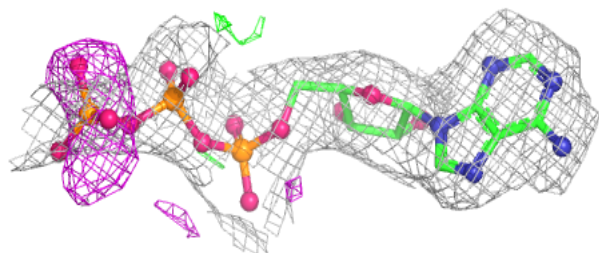
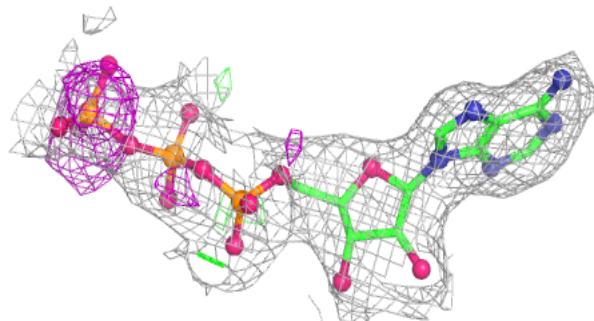
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	ATP	D	1004	31/31	0.89	0.13	30,40,81,82	0
2	ATP	C	1003	31/31	0.90	0.13	32,41,82,82	0
3	UGA	D	1104	37/37	0.90	0.15	31,36,61,62	0
2	ATP	B	1002	31/31	0.91	0.13	30,39,81,82	0
2	ATP	F	1006	31/31	0.91	0.14	27,40,81,82	0
3	UGA	C	1103	37/37	0.91	0.13	31,38,61,62	0
2	ATP	A	1001	31/31	0.91	0.13	28,39,82,83	0
3	UGA	F	1106	37/37	0.91	0.14	30,36,61,61	0
3	UGA	E	1105	37/37	0.92	0.14	30,36,60,61	0
2	ATP	E	1005	31/31	0.92	0.13	30,42,83,83	0
3	UGA	A	1101	37/37	0.93	0.15	27,36,61,61	0
3	UGA	B	1102	37/37	0.93	0.14	27,36,59,60	0

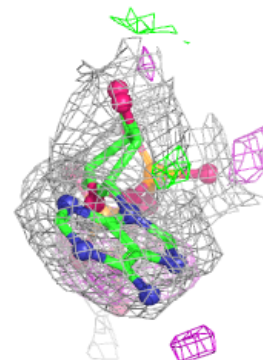
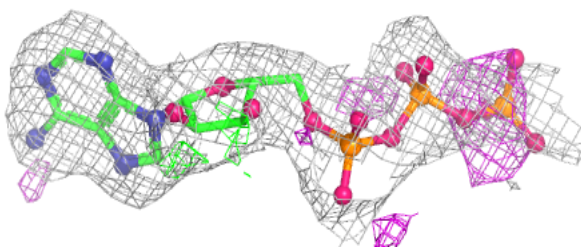
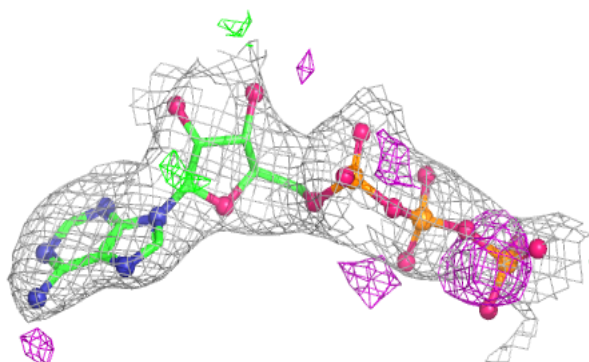
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ATP D 1004:

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

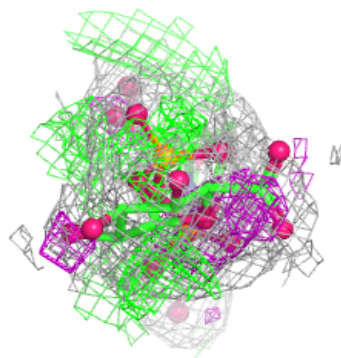
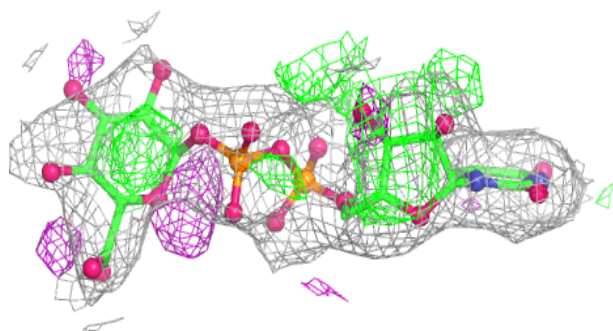
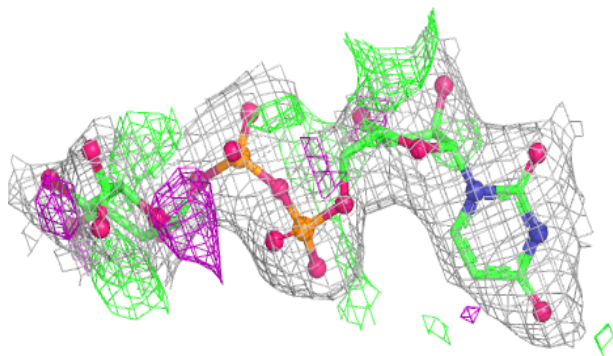
**Electron density around ATP C 1003:**

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

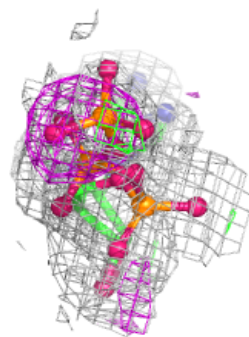
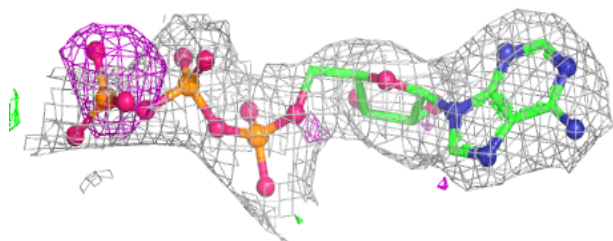
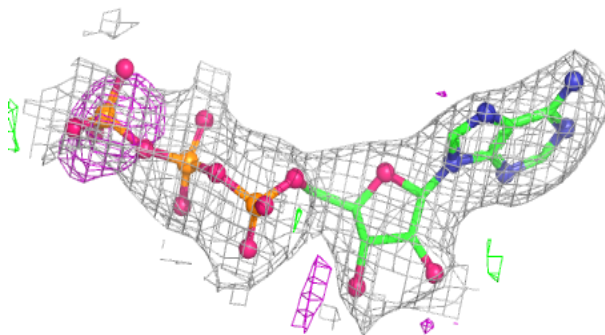


Electron density around UGA D 1104:

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

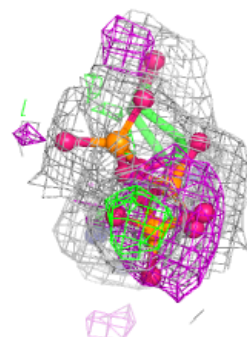
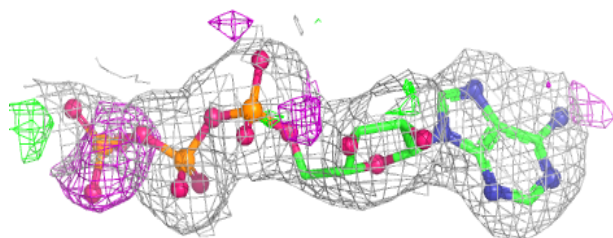
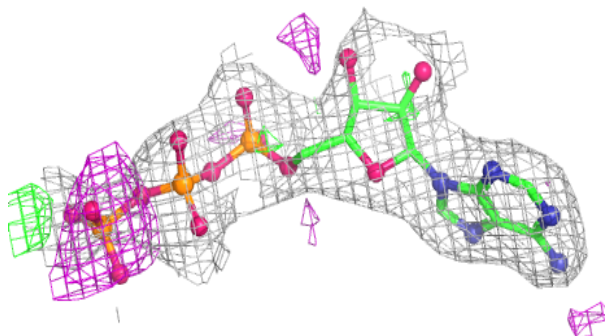
**Electron density around ATP B 1002:**

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

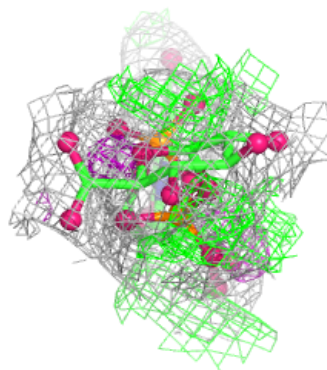
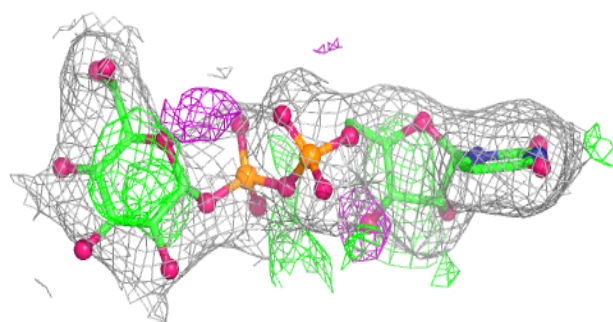
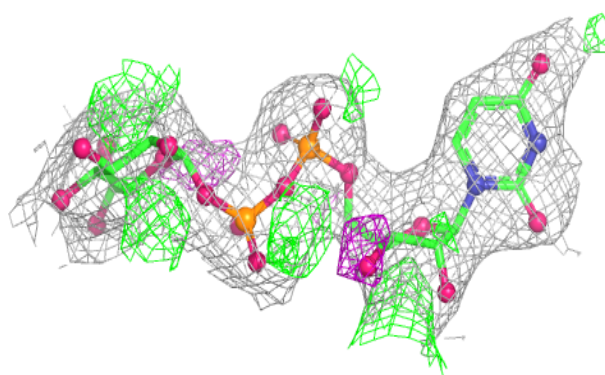


Electron density around ATP F 1006:

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

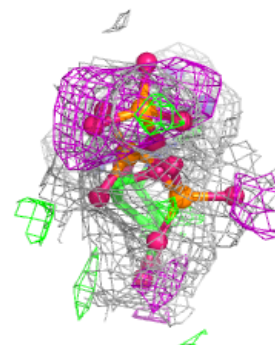
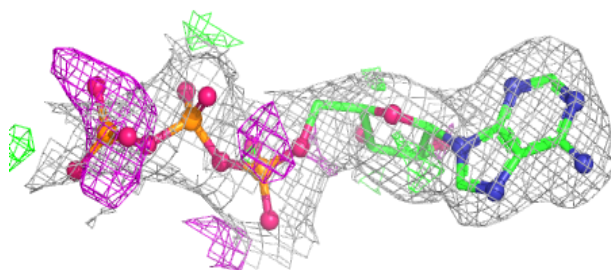
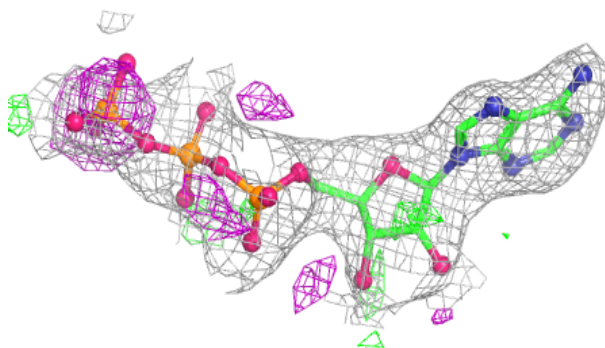
**Electron density around UGA C 1103:**

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

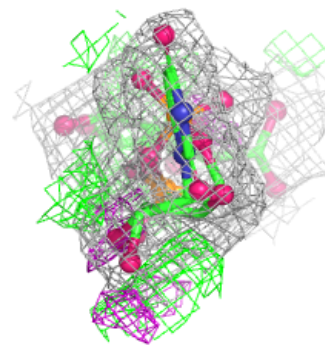
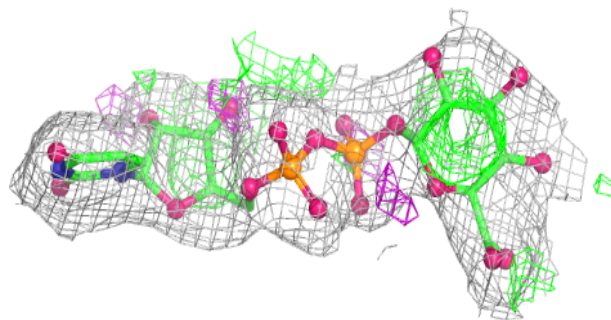
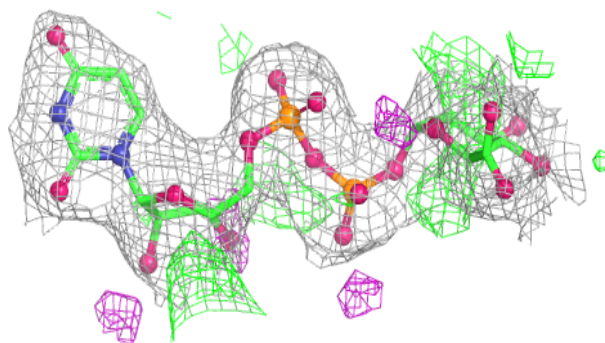


Electron density around ATP A 1001:

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

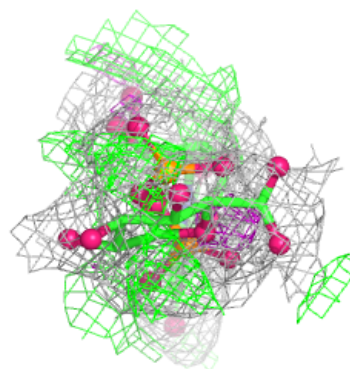
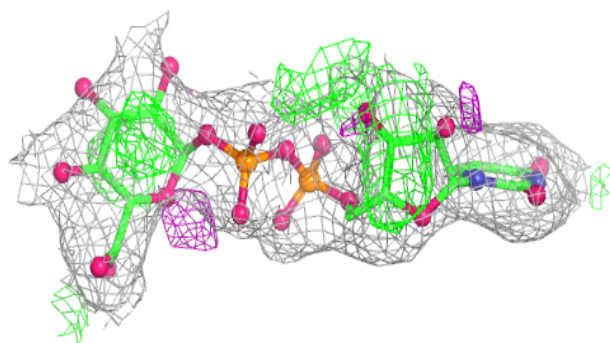
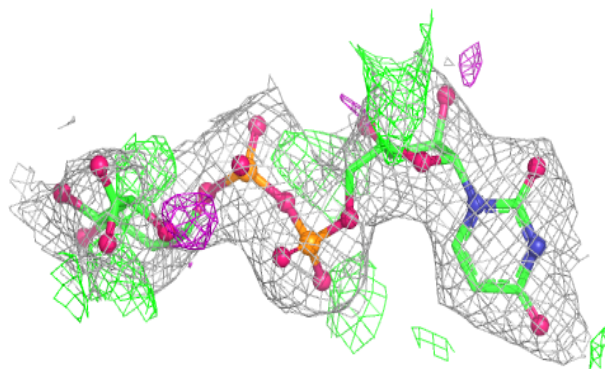
**Electron density around UGA F 1106:**

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

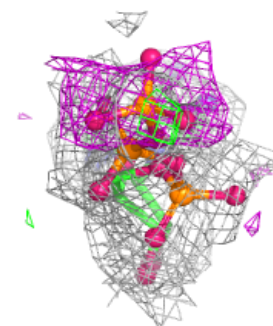
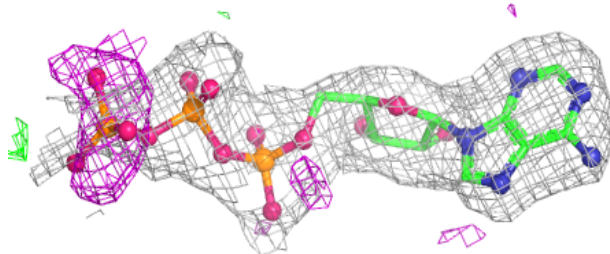
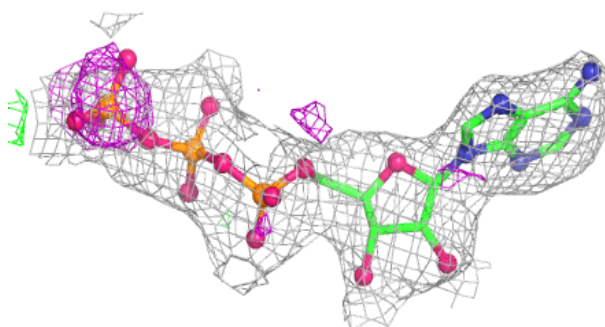


Electron density around UGA E 1105:

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

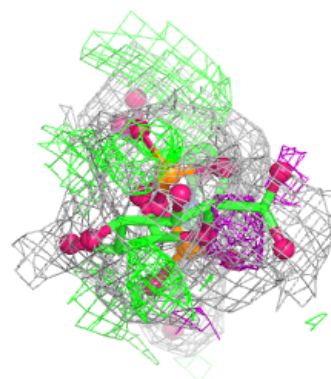
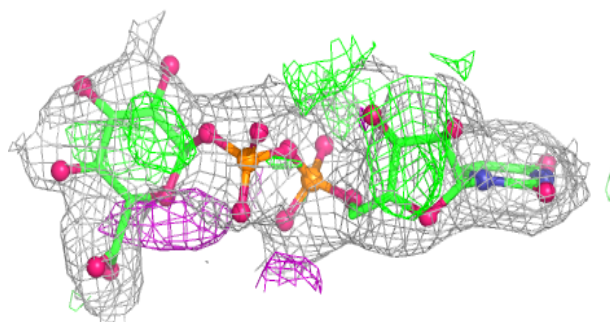
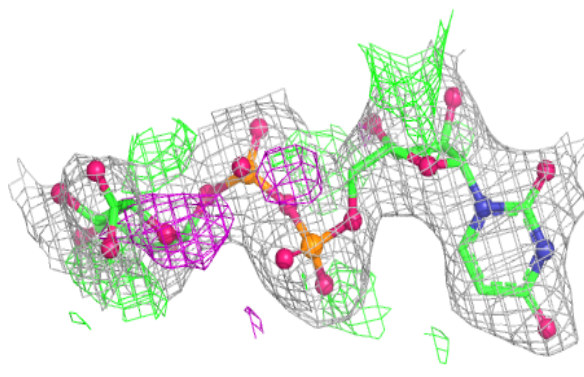
**Electron density around ATP E 1005:**

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

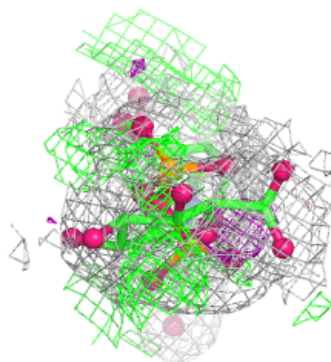
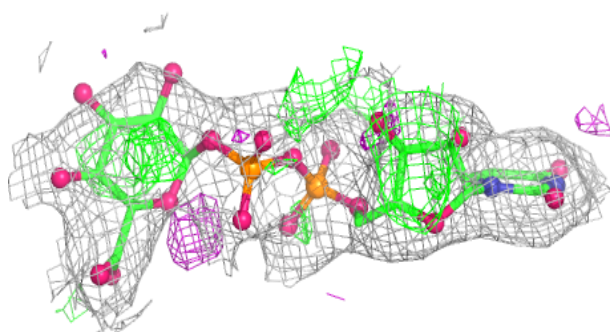
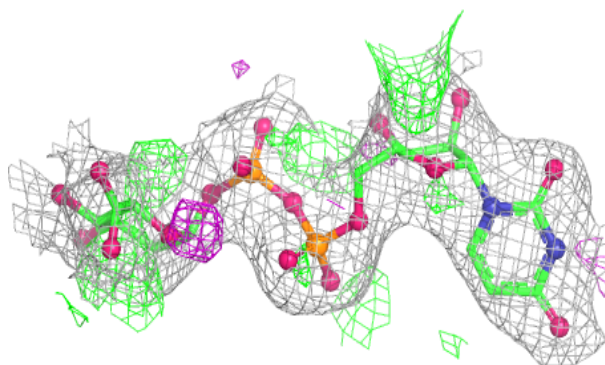


Electron density around UGA A 1101:

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

**Electron density around UGA B 1102:**

$2mF_o-DF_c$ (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.