



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:01 PM UTC

PDB ID : 8E5N / pdb_00008e5n
Title : Structure of ARG1 complex with pyrrolidine-based non-boronic acid inhibitor
10
Authors : Palte, R.L.; Gathiaka, S.
Deposited on : 2022-08-22
Resolution : 2.54 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

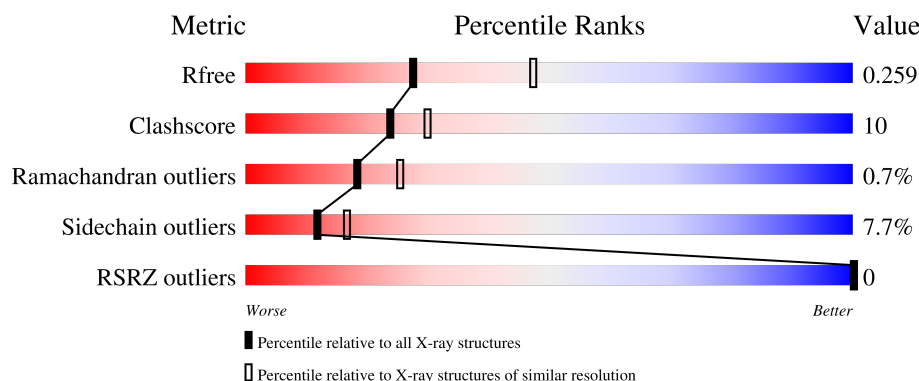
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	

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Mol	Chain	Length	Quality of chain
1	F	322	 72%22%••

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14716 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 Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	B	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	C	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	D	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	E	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			
1	F	317	Total	C	N	O	S	0	0	0
			2409	1535	411	457	6			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 1-{[(3S,4S)-3-(3-fluorophenyl)-4-{[4-(1,3,4-triethyl-1H-pyrazol-5-yl)piperidin-1-yl]methyl}pyrrolidin-1-yl]methyl}cyclopentane-1-carboxylic acid (CCD ID: UL0) (formula: C₃₂H₄₇FN₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 39	C 32	F 1	N 4	O 2	0	0
3	B	1	Total 39	C 32	F 1	N 4	O 2	0	0
3	C	1	Total 39	C 32	F 1	N 4	O 2	0	0
3	D	1	Total 39	C 32	F 1	N 4	O 2	0	0
3	E	1	Total 39	C 32	F 1	N 4	O 2	0	0
3	F	1	Total 39	C 32	F 1	N 4	O 2	0	0

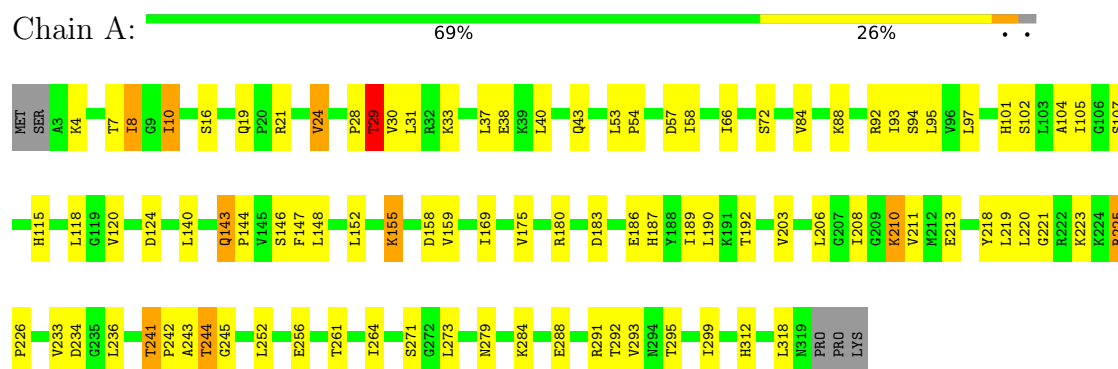
- Molecule 4 is water.

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

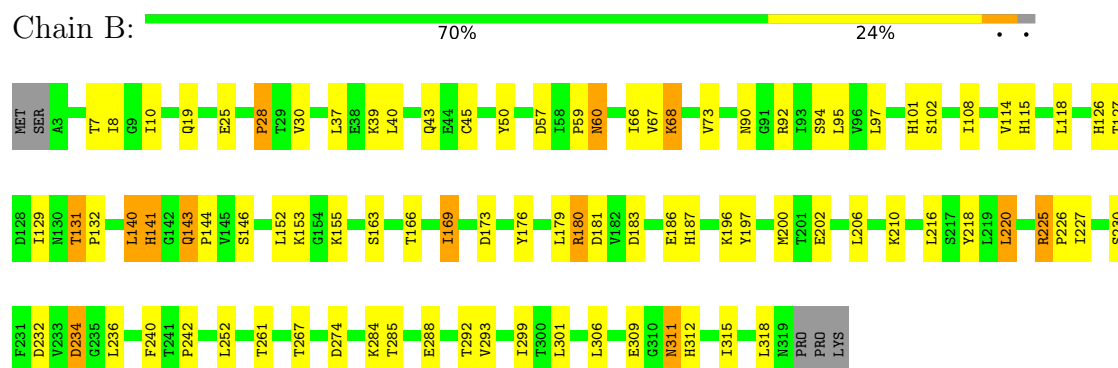
3 Residue-property plots

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

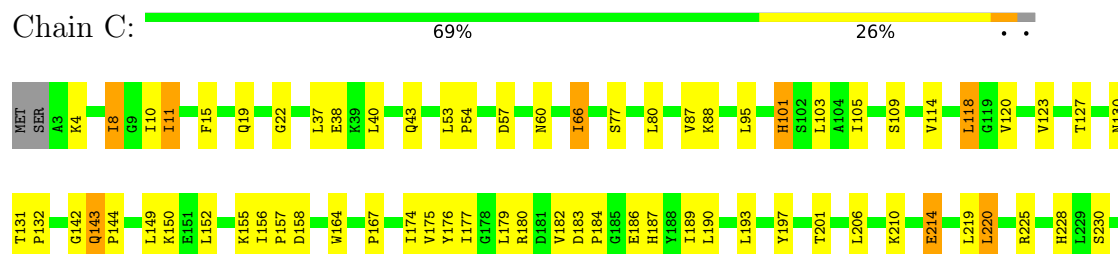
• Molecule 1: Arginase-1



• Molecule 1: Arginase-1



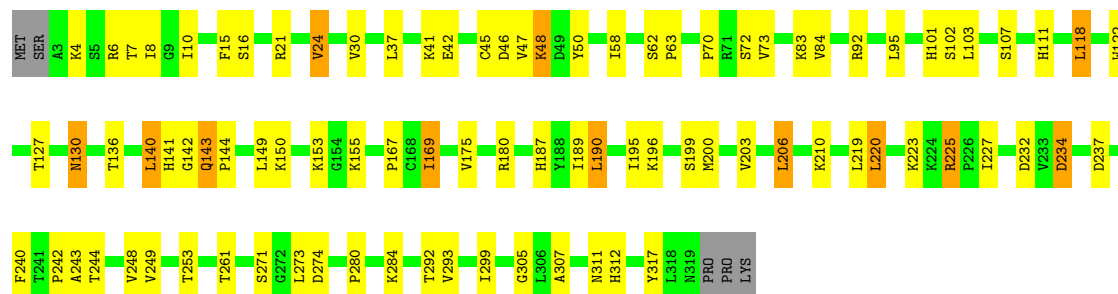
• Molecule 1: Arginase-1





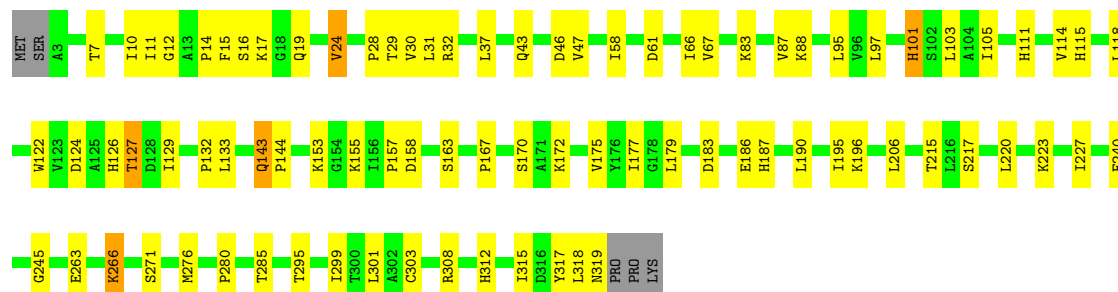
• Molecule 1: Arginase-1

Chain D: 70% 24%



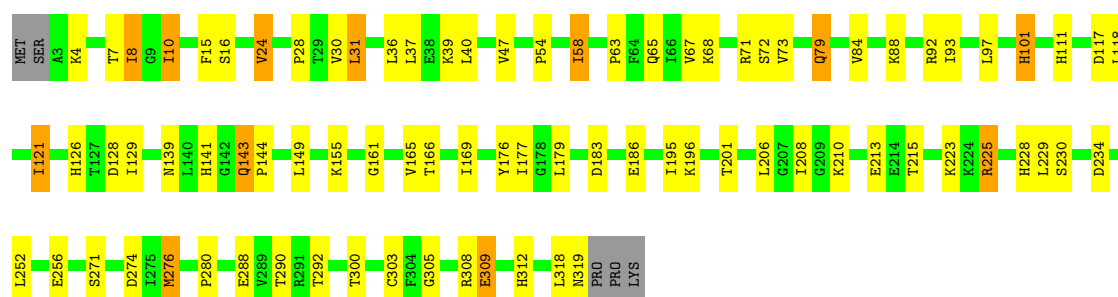
• Molecule 1: Arginase-1

Chain E: 72% 25%



• Molecule 1: Arginase-1

Chain F: 72% 22%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.42Å 287.54Å 67.35Å 90.00° 90.20° 90.00°	Depositor
Resolution (Å)	71.88 – 2.54 71.88 – 2.54	Depositor EDS
% Data completeness (in resolution range)	97.4 (71.88-2.54) 96.5 (71.88-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.55Å)	Xtriage
Refinement program	BUSTER 2.11.7 (20-MAY-2020)	Depositor
R, R_{free}	0.237 , 0.296 0.204 , 0.259	Depositor DCC
R_{free} test set	3192 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.913	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 3.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.349 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14716	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: UL0, MN

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	0.83	1/2459 (0.0%)	1.23	17/3336 (0.5%)
1	B	0.79	0/2459	1.22	10/3336 (0.3%)
1	C	0.83	1/2459 (0.0%)	1.21	9/3336 (0.3%)
1	D	0.78	0/2459	1.20	7/3336 (0.2%)
1	E	0.76	0/2459	1.14	5/3336 (0.1%)
1	F	0.77	0/2459	1.18	8/3336 (0.2%)
All	All	0.79	2/14754 (0.0%)	1.20	56/20016 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	315	ILE	CA-C	6.25	1.58	1.52
1	A	19	GLN	CA-C	5.54	1.57	1.52

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	ASP	CA-CB-CG	6.98	119.58	112.60
1	B	234	ASP	CA-CB-CG	6.87	119.47	112.60
1	A	245	GLY	N-CA-C	6.83	120.42	112.50
1	F	84	VAL	N-CA-C	-6.55	104.47	110.82
1	C	120	VAL	N-CA-C	6.31	117.88	108.54
1	B	68	LYS	CA-C-N	6.00	128.87	123.10
1	B	68	LYS	C-N-CA	6.00	128.87	123.10
1	B	311	ASN	CA-CB-CG	5.98	118.58	112.60
1	C	254	TYR	CA-C-N	5.98	128.54	120.65
1	C	254	TYR	C-N-CA	5.98	128.54	120.65
1	C	291	ARG	CA-C-N	5.92	128.21	120.28
1	C	291	ARG	C-N-CA	5.92	128.21	120.28
1	D	234	ASP	CA-CB-CG	5.76	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	THR	CA-C-N	5.74	128.33	120.46
1	A	29	THR	C-N-CA	5.74	128.33	120.46
1	A	10	ILE	N-CA-C	5.72	115.79	108.12
1	C	305	GLY	N-CA-C	5.71	121.57	114.37
1	E	245	GLY	N-CA-C	5.62	119.02	112.50
1	A	234	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	8	ILE	N-CA-C	5.50	116.41	108.48
1	B	220	LEU	CA-C-N	5.48	126.18	119.99
1	B	220	LEU	C-N-CA	5.48	126.18	119.99
1	E	105	ILE	N-CA-C	-5.43	105.31	110.42
1	A	244	THR	CA-C-N	5.42	125.96	119.94
1	A	244	THR	C-N-CA	5.42	125.96	119.94
1	D	45	CYS	CA-C-N	5.42	129.97	122.77
1	D	45	CYS	C-N-CA	5.42	129.97	122.77
1	D	274	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	60	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	21	ARG	CA-C-N	5.34	125.42	120.34
1	A	21	ARG	C-N-CA	5.34	125.42	120.34
1	D	253	THR	CA-C-N	5.29	127.32	120.44
1	D	253	THR	C-N-CA	5.29	127.32	120.44
1	F	305	GLY	N-CA-C	5.29	122.05	114.64
1	B	129	ILE	N-CA-CB	-5.28	104.38	112.15
1	A	158	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	120	VAL	N-CA-C	5.25	115.41	107.80
1	F	8	ILE	N-CA-C	5.22	116.83	108.89
1	F	276	MET	N-CA-C	5.20	118.03	109.72
1	B	28	PRO	CA-C-N	5.19	128.00	120.79
1	B	28	PRO	C-N-CA	5.19	128.00	120.79
1	F	28	PRO	CA-C-N	5.18	127.47	120.38
1	F	28	PRO	C-N-CA	5.18	127.47	120.38
1	C	276	MET	CA-C-N	5.17	129.90	122.35
1	C	276	MET	C-N-CA	5.17	129.90	122.35
1	E	163	SER	CA-C-N	5.14	129.43	120.68
1	E	163	SER	C-N-CA	5.14	129.43	120.68
1	C	22	GLY	N-CA-C	5.14	117.84	111.93
1	A	147	PHE	CA-C-N	5.12	128.09	120.31
1	A	147	PHE	C-N-CA	5.12	128.09	120.31
1	A	38	GLU	CA-C-N	5.10	127.12	120.28
1	A	38	GLU	C-N-CA	5.10	127.12	120.28
1	E	240	PHE	CA-CB-CG	-5.06	108.74	113.80
1	F	234	ASP	CA-CB-CG	5.06	117.66	112.60
1	D	130	ASN	CA-CB-CG	5.02	117.62	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	165	VAL	N-CA-C	5.02	115.51	108.89

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	2409	0	2456	52	0
1	B	2409	0	2456	49	0
1	C	2409	0	2456	58	0
1	D	2409	0	2456	59	0
1	E	2409	0	2456	48	0
1	F	2409	0	2456	53	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	39	0	0	0	0
3	B	39	0	0	0	0
3	C	39	0	0	1	0
3	D	39	0	0	0	0
3	E	39	0	0	0	0
3	F	39	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	14716	0	14736	298	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (298) 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:11:ILE:HD11	1:E:87:VAL:HG21	1.41	1.03
1:A:30:VAL:HA	1:A:33:LYS:HD2	1.47	0.94
1:D:102:SER:HA	1:D:144:PRO:HG3	1.52	0.92
1:E:88:LYS:NZ	1:E:271:SER:HB3	1.90	0.87
1:F:88:LYS:NZ	1:F:271:SER:HB3	1.89	0.87
1:C:88:LYS:NZ	1:C:271:SER:HB3	1.90	0.85
1:C:210:LYS:NZ	1:C:214:GLU:HB2	1.92	0.85
1:A:288:GLU:HG2	1:A:291:ARG:HH21	1.40	0.83
1:F:223:LYS:NZ	1:F:225:ARG:HB3	1.97	0.80
1:A:187:HIS:CE1	1:B:312:HIS:HD1	2.00	0.79
1:D:307:ALA:H	1:D:311:ASN:HD21	1.31	0.78
1:F:230:SER:HA	1:F:274:ASP:HB2	1.65	0.78
1:C:210:LYS:HZ3	1:C:214:GLU:HB2	1.48	0.78
1:A:187:HIS:ND1	1:B:312:HIS:ND1	2.27	0.78
1:C:43:GLN:OE1	1:C:306:LEU:HB2	1.84	0.77
1:C:88:LYS:HZ1	1:C:271:SER:HB3	1.51	0.76
1:B:187:HIS:ND1	1:E:312:HIS:ND1	2.32	0.76
1:F:15:PHE:HZ	1:F:73:VAL:HG22	1.51	0.76
1:F:93:ILE:HG12	1:F:271:SER:HA	1.67	0.75
1:F:223:LYS:HZ3	1:F:225:ARG:HB3	1.55	0.71
1:F:88:LYS:HZ3	1:F:271:SER:HB3	1.54	0.71
1:D:102:SER:HB3	1:D:141:HIS:HA	1.73	0.70
1:D:143:GLN:H	1:D:144:PRO:CD	2.05	0.70
1:E:295:THR:O	1:E:299:ILE:HG12	1.92	0.69
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.76	0.68
1:F:88:LYS:HZ1	1:F:271:SER:HB3	1.57	0.68
1:A:30:VAL:HA	1:A:33:LYS:CD	2.24	0.68
1:A:4:LYS:O	1:A:93:ILE:HD11	1.94	0.68
1:E:88:LYS:HZ1	1:E:271:SER:HB3	1.58	0.68
1:B:114:VAL:HG12	1:B:115:HIS:CD2	2.30	0.67
1:E:114:VAL:HG12	1:E:115:HIS:CD2	2.31	0.65
1:E:88:LYS:HZ3	1:E:271:SER:HB3	1.60	0.64
1:A:16:SER:HB2	1:A:24:VAL:HG12	1.78	0.63
1:B:30:VAL:HG12	1:B:293:VAL:HG21	1.80	0.63
1:A:210:LYS:NZ	1:A:213:GLU:HB3	2.12	0.63
1:D:16:SER:HB2	1:D:24:VAL:HG12	1.79	0.63
1:D:242:PRO:HD2	1:D:292:THR:OG1	1.99	0.62
1:C:143:GLN:N	1:C:144:PRO:HD2	2.15	0.62
1:B:216:LEU:HD22	1:B:267:THR:HG21	1.82	0.62
1:F:101:HIS:CD2	1:F:276:MET:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:GLN:H	1:C:144:PRO:HD2	1.65	0.61
1:B:236:LEU:HD23	1:B:252:LEU:HB2	1.83	0.61
1:D:84:VAL:HG21	1:D:107:SER:HA	1.83	0.61
1:C:8:ILE:HD13	1:C:40:LEU:HD13	1.83	0.60
1:E:127:THR:HB	1:E:129:ILE:HG22	1.83	0.60
1:C:15:PHE:HB3	1:C:103:LEU:HD21	1.83	0.60
1:C:150:LYS:HA	1:C:167:PRO:HB2	1.84	0.60
1:A:210:LYS:HA	1:A:213:GLU:HB2	1.83	0.60
1:F:121:ILE:HG22	1:F:229:LEU:HD13	1.84	0.59
1:F:31:LEU:HD22	1:F:36:LEU:HD22	1.84	0.59
1:F:143:GLN:N	1:F:144:PRO:HD2	2.17	0.59
1:B:169:ILE:HG22	1:B:173:ASP:HB2	1.85	0.59
1:C:152:LEU:HD23	1:C:155:LYS:HG3	1.86	0.58
1:A:242:PRO:HB3	1:A:284:LYS:HZ3	1.69	0.58
1:A:10:ILE:HG21	1:A:37:LEU:HD11	1.86	0.57
1:D:16:SER:CB	1:D:24:VAL:HG12	2.35	0.57
1:D:220:LEU:HD11	1:D:227:ILE:HD11	1.87	0.57
1:E:111:HIS:CE1	1:E:271:SER:HB2	2.39	0.57
1:D:130:ASN:HB2	1:D:142:GLY:O	2.05	0.57
1:D:187:HIS:NE2	1:F:309:GLU:OE2	2.37	0.57
1:C:130:ASN:HB2	1:C:142:GLY:O	2.06	0.56
1:E:127:THR:HG23	1:E:179:LEU:CD2	2.35	0.56
1:E:312:HIS:HB2	1:E:317:TYR:CE2	2.40	0.56
1:A:105:ILE:HA	1:A:148:LEU:HD21	1.86	0.56
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.88	0.56
1:C:88:LYS:HZ3	1:C:271:SER:HB3	1.66	0.56
1:E:220:LEU:HD11	1:E:227:ILE:HD11	1.86	0.56
1:D:15:PHE:HB3	1:D:103:LEU:HD11	1.87	0.56
1:F:15:PHE:CZ	1:F:73:VAL:HG22	2.37	0.56
1:C:11:ILE:HD11	1:C:87:VAL:HG21	1.87	0.56
1:D:7:THR:HA	1:D:46:ASP:HB3	1.87	0.56
1:D:155:LYS:HZ1	1:F:319:ASN:ND2	2.03	0.55
1:F:223:LYS:HZ2	1:F:225:ARG:HB3	1.71	0.55
1:F:10:ILE:HG21	1:F:37:LEU:HD11	1.89	0.55
1:C:210:LYS:HZ1	1:C:214:GLU:HB2	1.69	0.55
1:E:127:THR:HG23	1:E:179:LEU:HD21	1.87	0.55
1:A:203:VAL:HG22	1:A:211:VAL:HG21	1.89	0.55
1:D:95:LEU:HD13	1:D:273:LEU:HD23	1.87	0.55
1:B:187:HIS:ND1	1:E:312:HIS:CE1	2.75	0.54
1:C:143:GLN:H	1:C:144:PRO:CD	2.20	0.54
1:B:176:TYR:HB3	1:B:179:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:HIS:HB3	1:A:226:PRO:HG2	1.89	0.54
1:E:129:ILE:HG23	1:E:129:ILE:O	2.08	0.54
1:B:50:TYR:OH	1:B:90:ASN:ND2	2.41	0.54
1:B:114:VAL:HG12	1:B:115:HIS:NE2	2.22	0.54
1:F:31:LEU:HD13	1:F:97:LEU:HD22	1.90	0.54
1:D:206:LEU:HB2	1:D:210:LYS:HB3	1.90	0.53
1:F:71:ARG:HA	1:F:161:GLY:HA3	1.90	0.53
1:C:10:ILE:HD12	1:C:37:LEU:HG	1.90	0.53
1:F:139:ASN:HB3	1:F:141:HIS:HD2	1.73	0.53
1:D:30:VAL:HG12	1:D:293:VAL:HG21	1.90	0.53
1:D:63:PRO:HA	1:D:70:PRO:HD3	1.90	0.53
1:C:80:LEU:HD22	1:C:103:LEU:HB3	1.90	0.53
1:D:175:VAL:HG22	1:D:196:LYS:HB3	1.91	0.52
1:B:25:GLU:O	1:B:28:PRO:HD2	2.10	0.52
1:A:219:LEU:O	1:A:225:ARG:HD2	2.10	0.52
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.46	0.51
1:E:101:HIS:O	1:E:144:PRO:HG3	2.11	0.51
1:C:236:LEU:HA	1:C:252:LEU:HB2	1.92	0.51
1:A:8:ILE:HD13	1:A:40:LEU:HD13	1.91	0.51
1:A:95:LEU:HD13	1:A:273:LEU:HD23	1.93	0.51
1:E:7:THR:HA	1:E:46:ASP:HB3	1.93	0.51
1:F:176:TYR:HB3	1:F:179:LEU:HD11	1.93	0.51
1:F:177:ILE:HD11	1:F:215:THR:HG21	1.93	0.51
1:A:210:LYS:NZ	1:A:213:GLU:CB	2.74	0.51
1:C:101:HIS:NE2	1:C:230:SER:OG	2.31	0.51
1:C:206:LEU:HB3	1:C:210:LYS:HB3	1.91	0.51
1:B:40:LEU:O	1:B:45:CYS:HB2	2.10	0.50
1:D:102:SER:HA	1:D:144:PRO:CG	2.32	0.50
1:C:289:VAL:O	1:C:293:VAL:HG23	2.11	0.50
1:C:187:HIS:ND1	1:D:312:HIS:ND1	2.59	0.50
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.93	0.50
1:A:208:ILE:HB	1:A:256:GLU:HG2	1.94	0.50
1:B:176:TYR:HB2	1:B:197:TYR:HA	1.93	0.50
1:B:39:LYS:HB3	1:B:301:LEU:HD21	1.94	0.50
1:B:102:SER:HB3	1:B:141:HIS:HA	1.94	0.50
1:E:31:LEU:HD13	1:E:97:LEU:HD22	1.92	0.50
1:F:63:PRO:HB3	1:F:68:LYS:HA	1.94	0.49
1:B:101:HIS:ND1	1:B:232:ASP:HB2	2.27	0.49
1:D:48:LYS:HB2	1:D:92:ARG:CZ	2.42	0.49
1:B:59:PRO:O	1:B:60:ASN:HB2	2.12	0.49
1:C:182:VAL:HG13	1:C:186:GLU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:HIS:CE1	1:D:122:TRP:NE1	2.81	0.49
1:A:102:SER:HA	1:A:144:PRO:HG3	1.95	0.49
1:A:187:HIS:CE1	1:B:312:HIS:ND1	2.74	0.49
1:F:16:SER:CB	1:F:24:VAL:HG12	2.43	0.49
1:B:108:ILE:HG21	1:B:169:ILE:HD11	1.95	0.49
1:B:126:HIS:CD2	1:B:181:ASP:HB3	2.48	0.49
1:A:143:GLN:O	1:A:146:SER:OG	2.30	0.49
1:A:242:PRO:HB3	1:A:284:LYS:NZ	2.28	0.49
1:C:105:ILE:O	1:C:109:SER:OG	2.28	0.49
1:D:143:GLN:N	1:D:144:PRO:CD	2.75	0.49
1:A:206:LEU:O	1:A:210:LYS:HB3	2.12	0.48
1:C:123:VAL:HG22	1:C:177:ILE:HB	1.94	0.48
1:B:10:ILE:HD12	1:B:95:LEU:HD23	1.95	0.48
1:E:122:TRP:CD1	1:E:124:ASP:HB2	2.48	0.48
1:E:16:SER:CB	1:E:24:VAL:HG12	2.43	0.48
1:D:261:THR:HG21	1:D:299:ILE:HG23	1.95	0.48
1:E:10:ILE:HG13	1:E:37:LEU:HD11	1.96	0.48
1:D:143:GLN:H	1:D:144:PRO:HD3	1.79	0.48
1:E:133:LEU:HD21	1:E:157:PRO:HG3	1.94	0.48
1:F:16:SER:HB3	1:F:24:VAL:HG12	1.95	0.48
1:A:31:LEU:HD23	1:A:293:VAL:HG13	1.95	0.47
1:B:200:MET:HB2	1:E:308:ARG:HD2	1.97	0.47
1:C:95:LEU:HD13	1:C:273:LEU:HD23	1.96	0.47
1:D:237:ASP:HB3	1:D:240:PHE:CD2	2.49	0.47
1:C:143:GLN:N	1:C:144:PRO:CD	2.77	0.47
1:D:149:LEU:HD23	1:D:169:ILE:HD12	1.96	0.47
1:E:16:SER:HB2	1:E:24:VAL:HG12	1.96	0.47
1:F:176:TYR:CB	1:F:179:LEU:HD11	2.44	0.47
1:A:183:ASP:HB2	1:A:186:GLU:HG3	1.95	0.47
1:A:295:THR:O	1:A:299:ILE:HG12	2.15	0.47
1:A:241:THR:HG22	1:A:292:THR:HG23	1.97	0.47
1:B:7:THR:HG22	1:B:92:ARG:HG2	1.96	0.47
1:B:146:SER:HA	1:B:152:LEU:HD12	1.97	0.47
1:F:143:GLN:N	1:F:144:PRO:CD	2.76	0.47
1:A:29:THR:O	1:A:33:LYS:HG3	2.14	0.47
1:D:41:LYS:NZ	1:D:47:VAL:HB	2.29	0.47
1:E:124:ASP:HB3	1:E:126:HIS:O	2.15	0.47
1:A:143:GLN:H	1:A:144:PRO:HD3	1.79	0.47
1:C:152:LEU:HB3	1:C:156:ILE:HD11	1.97	0.47
1:F:7:THR:HG22	1:F:92:ARG:HG2	1.96	0.47
1:D:48:LYS:NZ	1:D:50:TYR:CE2	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:228:HIS:C	1:F:228:HIS:CD2	2.92	0.46
1:E:28:PRO:O	1:E:32:ARG:HG3	2.15	0.46
1:E:143:GLN:N	1:E:144:PRO:CD	2.79	0.46
1:A:243:ALA:HB1	1:A:279:ASN:O	2.16	0.46
1:C:280:PRO:HA	1:C:289:VAL:HG13	1.97	0.46
1:F:8:ILE:HD13	1:F:40:LEU:HD13	1.97	0.46
1:A:220:LEU:HD23	1:A:225:ARG:HG3	1.95	0.46
1:E:103:LEU:HB2	1:E:276:MET:HE1	1.97	0.46
1:A:7:THR:HG22	1:A:92:ARG:HG2	1.97	0.46
1:D:155:LYS:HZ1	1:F:319:ASN:HD21	1.62	0.46
1:B:155:LYS:HD2	1:E:318:LEU:HB3	1.96	0.46
1:D:10:ILE:HD12	1:D:95:LEU:HD23	1.98	0.46
1:D:150:LYS:HA	1:D:167:PRO:HB2	1.96	0.46
1:F:10:ILE:HG13	1:F:47:VAL:HG13	1.96	0.46
1:D:189:ILE:HG12	1:F:318:LEU:HD11	1.97	0.46
1:C:243:ALA:HA	1:C:282:LEU:O	2.15	0.46
1:C:40:LEU:HD23	1:C:301:LEU:HD23	1.96	0.45
1:A:143:GLN:N	1:A:144:PRO:CD	2.79	0.45
1:C:150:LYS:HA	1:C:167:PRO:CB	2.45	0.45
1:C:184:PRO:HA	1:D:311:ASN:O	2.16	0.45
1:E:111:HIS:NE2	1:E:271:SER:HB2	2.32	0.45
1:D:58:ILE:HD12	1:D:72:SER:HA	1.98	0.45
1:F:129:ILE:HD11	1:F:149:LEU:HD11	1.98	0.45
1:A:16:SER:CB	1:A:24:VAL:HG12	2.45	0.45
1:D:237:ASP:HB3	1:D:240:PHE:HD2	1.80	0.45
1:C:189:ILE:O	1:C:193:LEU:HB2	2.17	0.45
1:E:187:HIS:CD2	1:E:190:LEU:HD23	2.51	0.45
1:A:233:VAL:HB	1:A:241:THR:HG21	1.98	0.45
1:B:73:VAL:HG11	1:B:140:LEU:HB3	1.98	0.45
1:D:143:GLN:H	1:D:144:PRO:HD2	1.81	0.45
1:F:30:VAL:HG21	1:F:280:PRO:HG3	1.98	0.45
1:A:88:LYS:NZ	1:A:271:SER:HB3	2.32	0.45
1:B:43:GLN:OE1	1:B:306:LEU:HB2	2.17	0.45
1:A:236:LEU:HA	1:A:252:LEU:HB2	1.98	0.45
1:C:66:ILE:HD12	1:C:66:ILE:HA	1.93	0.45
1:D:199:SER:O	1:D:203:VAL:HG23	2.17	0.45
1:E:143:GLN:N	1:E:144:PRO:HD2	2.31	0.45
1:F:149:LEU:HD23	1:F:169:ILE:HG13	1.99	0.44
1:F:223:LYS:NZ	1:F:225:ARG:CB	2.76	0.44
1:C:183:ASP:HB2	1:C:186:GLU:HG3	1.99	0.44
1:D:200:MET:HB2	1:F:308:ARG:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ASP:HB3	1:D:244:THR:HG21	1.99	0.44
1:F:54:PRO:O	1:F:79:GLN:OE1	2.35	0.44
1:B:183:ASP:HB2	1:B:186:GLU:HG3	1.98	0.44
1:D:73:VAL:HB	1:D:140:LEU:HD13	1.99	0.44
1:D:155:LYS:NZ	1:F:319:ASN:ND2	2.66	0.44
1:E:15:PHE:HB3	1:E:103:LEU:HD11	1.99	0.44
1:A:104:ALA:HA	1:A:107:SER:HB2	2.00	0.44
1:D:37:LEU:HG	1:D:47:VAL:HG11	2.00	0.44
1:B:114:VAL:CG1	1:B:115:HIS:NE2	2.80	0.44
1:C:318:LEU:HB3	1:F:155:LYS:HD2	1.99	0.44
1:D:187:HIS:ND1	1:F:312:HIS:ND1	2.64	0.44
1:C:132:PRO:HD2	1:C:157:PRO:HD2	1.99	0.44
1:F:183:ASP:HB2	1:F:186:GLU:HG3	1.99	0.44
1:A:192:THR:HG22	1:C:158:ASP:HB3	2.00	0.43
1:D:111:HIS:CG	1:D:118:LEU:HD22	2.53	0.43
1:D:190:LEU:HD12	1:D:195:ILE:HB	2.00	0.43
1:B:240:PHE:C	1:B:242:PRO:HD3	2.43	0.43
1:C:190:LEU:HG	1:C:197:TYR:CD1	2.53	0.43
1:E:183:ASP:HB2	1:E:186:GLU:HG3	2.01	0.43
1:A:189:ILE:HD11	1:B:318:LEU:HD21	1.99	0.43
1:E:190:LEU:HD12	1:E:195:ILE:HB	2.01	0.43
1:B:131:THR:HG22	1:B:146:SER:HB2	2.00	0.43
1:C:279:ASN:HB3	1:C:282:LEU:HB2	2.01	0.43
1:F:8:ILE:HD12	1:F:47:VAL:HG22	2.01	0.43
1:F:288:GLU:O	1:F:292:THR:OG1	2.28	0.43
1:B:143:GLN:N	1:B:144:PRO:CD	2.82	0.43
1:E:187:HIS:HD2	1:E:190:LEU:HD23	1.83	0.43
1:B:30:VAL:CG1	1:B:293:VAL:HG21	2.45	0.43
1:B:114:VAL:CG1	1:B:115:HIS:CD2	3.00	0.43
1:B:180:ARG:HB3	1:B:200:MET:HG2	2.01	0.43
1:C:38:GLU:N	1:C:38:GLU:CD	2.77	0.43
1:C:164:TRP:H	1:C:164:TRP:CD1	2.35	0.43
1:E:153:LYS:HG3	1:E:167:PRO:HG2	2.01	0.43
1:C:149:LEU:HD12	1:C:152:LEU:HD12	1.99	0.43
1:E:12:GLY:O	1:E:14:PRO:HD3	2.19	0.43
1:F:58:ILE:HD13	1:F:72:SER:HA	2.01	0.43
1:F:206:LEU:HB3	1:F:210:LYS:HB3	2.01	0.43
1:C:183:ASP:OD1	3:C:1003:UL0:N3	2.51	0.43
1:D:127:THR:HG21	1:D:190:LEU:HD22	2.00	0.43
1:E:67:VAL:HG21	1:E:132:PRO:HA	2.01	0.43
1:A:58:ILE:HD13	1:A:72:SER:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:HIS:CE1	1:D:122:TRP:CE2	3.07	0.42
1:F:208:ILE:HB	1:F:256:GLU:HG2	2.00	0.42
1:A:242:PRO:CB	1:A:284:LYS:NZ	2.82	0.42
1:B:225:ARG:H	1:B:225:ARG:HG3	1.56	0.42
1:B:288:GLU:O	1:B:292:THR:OG1	2.30	0.42
1:A:318:LEU:HD13	1:E:155:LYS:HG3	2.01	0.42
1:F:139:ASN:HB3	1:F:141:HIS:CD2	2.54	0.42
1:D:101:HIS:CE1	1:D:232:ASP:HB2	2.55	0.42
1:E:43:GLN:OE1	1:E:301:LEU:HB3	2.19	0.42
1:B:200:MET:HE1	1:B:252:LEU:HD23	2.01	0.42
1:C:88:LYS:HB2	1:C:114:VAL:HG21	2.02	0.42
1:C:105:ILE:O	1:C:109:SER:CB	2.67	0.42
1:C:118:LEU:HD13	1:C:228:HIS:HB2	2.01	0.42
1:C:15:PHE:CB	1:C:103:LEU:HD21	2.49	0.42
1:A:175:VAL:HG22	1:A:218:TYR:CE2	2.55	0.42
1:A:155:LYS:NZ	1:C:60:ASN:HB2	2.34	0.42
1:C:300:THR:O	1:C:303:CYS:HB2	2.20	0.42
1:C:176:TYR:HB3	1:C:179:LEU:HD21	2.02	0.42
1:D:150:LYS:HA	1:D:167:PRO:CB	2.50	0.42
1:C:240:PHE:HE2	1:C:253:THR:HG22	1.85	0.41
1:F:126:HIS:HB2	1:F:128:ASP:OD1	2.19	0.41
1:D:312:HIS:HB2	1:D:317:TYR:CE2	2.55	0.41
1:E:263:GLU:HA	1:E:266:LYS:HG3	2.02	0.41
1:B:230:SER:HA	1:B:274:ASP:HB2	2.01	0.41
1:D:83:LYS:HA	1:D:83:LYS:HD3	1.89	0.41
1:D:243:ALA:HB3	1:D:292:THR:HG21	2.03	0.41
1:B:67:VAL:HG21	1:B:132:PRO:HB3	2.02	0.41
1:B:126:HIS:HE1	1:B:234:ASP:OD2	2.04	0.41
1:D:219:LEU:O	1:D:225:ARG:NH1	2.54	0.41
1:A:53:LEU:HA	1:A:54:PRO:HD3	1.98	0.41
1:C:180:ARG:CZ	1:C:251:GLY:HA3	2.51	0.41
1:A:84:VAL:HG21	1:A:107:SER:HA	2.02	0.41
1:C:53:LEU:HA	1:C:54:PRO:HD3	1.93	0.41
1:C:175:VAL:HG23	1:C:219:LEU:HD21	2.02	0.41
1:D:30:VAL:HG21	1:D:280:PRO:HG3	2.03	0.41
1:C:220:LEU:HD13	1:C:269:LEU:HD12	2.03	0.41
1:E:170:SER:C	1:E:172:LYS:H	2.29	0.41
1:A:206:LEU:HB3	1:A:210:LYS:HG2	2.03	0.40
1:E:83:LYS:HA	1:E:83:LYS:HD3	1.93	0.40
1:B:196:LYS:HB2	1:B:218:TYR:CZ	2.56	0.40
1:D:180:ARG:HG3	1:D:248:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:30:VAL:HG21	1:E:280:PRO:HG3	2.03	0.40
1:F:117:ASP:HB2	1:F:223:LYS:NZ	2.36	0.40
1:F:252:LEU:HD22	1:F:256:GLU:HB3	2.03	0.40
1:B:115:HIS:HB3	1:B:226:PRO:HG2	2.03	0.40
1:D:6:ARG:HH21	1:D:305:GLY:HA3	1.84	0.40
1:E:175:VAL:HG11	1:E:215:THR:HG23	2.03	0.40
1:E:175:VAL:HG22	1:E:196:LYS:HB3	2.03	0.40
1:F:111:HIS:CG	1:F:118:LEU:HD22	2.56	0.40
1:A:28:PRO:HG3	1:A:97:LEU:O	2.22	0.40
1:A:140:LEU:O	1:A:144:PRO:HD3	2.22	0.40
1:D:140:LEU:O	1:D:144:PRO:HD3	2.21	0.40
1:E:58:ILE:HG22	1:E:61:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	315/322 (98%)	289 (92%)	23 (7%)	3 (1%)	12	17
1	B	315/322 (98%)	290 (92%)	22 (7%)	3 (1%)	12	17
1	C	315/322 (98%)	301 (96%)	12 (4%)	2 (1%)	21	29
1	D	315/322 (98%)	293 (93%)	20 (6%)	2 (1%)	21	29
1	E	315/322 (98%)	287 (91%)	27 (9%)	1 (0%)	36	45
1	F	315/322 (98%)	299 (95%)	13 (4%)	3 (1%)	12	17
All	All	1890/1932 (98%)	1759 (93%)	117 (6%)	14 (1%)	18	25

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	195	ILE

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Mol	Chain	Res	Type
1	A	221	GLY
1	D	143	GLN
1	A	180	ARG
1	B	57	ASP
1	C	143	GLN
1	D	4	LYS
1	F	67	VAL
1	B	143	GLN
1	B	180	ARG
1	C	252	LEU
1	A	143	GLN
1	E	143	GLN
1	F	143	GLN

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	265/270 (98%)	245 (92%)	20 (8%)	12	17
1	B	265/270 (98%)	240 (91%)	25 (9%)	8	10
1	C	265/270 (98%)	245 (92%)	20 (8%)	12	17
1	D	265/270 (98%)	246 (93%)	19 (7%)	13	18
1	E	265/270 (98%)	245 (92%)	20 (8%)	12	17
1	F	265/270 (98%)	246 (93%)	19 (7%)	13	18
All	All	1590/1620 (98%)	1467 (92%)	123 (8%)	12	17

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	29	THR
1	A	43	GLN
1	A	57	ASP
1	A	66	ILE

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Mol	Chain	Res	Type
1	A	94	SER
1	A	101	HIS
1	A	118	LEU
1	A	152	LEU
1	A	155	LYS
1	A	159	VAL
1	A	169	ILE
1	A	190	LEU
1	A	210	LYS
1	A	223	LYS
1	A	225	ARG
1	A	241	THR
1	A	244	THR
1	A	264	ILE
1	A	312	HIS
1	B	8	ILE
1	B	19	GLN
1	B	37	LEU
1	B	66	ILE
1	B	68	LYS
1	B	94	SER
1	B	97	LEU
1	B	118	LEU
1	B	127	THR
1	B	131	THR
1	B	140	LEU
1	B	141	HIS
1	B	153	LYS
1	B	163	SER
1	B	166	THR
1	B	169	ILE
1	B	202	GLU
1	B	206	LEU
1	B	210	LYS
1	B	225	ARG
1	B	284	LYS
1	B	285	THR
1	B	309	GLU
1	B	311	ASN
1	B	315	ILE
1	C	4	LYS
1	C	8	ILE

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Mol	Chain	Res	Type
1	C	11	ILE
1	C	19	GLN
1	C	57	ASP
1	C	66	ILE
1	C	77	SER
1	C	101	HIS
1	C	118	LEU
1	C	127	THR
1	C	131	THR
1	C	174	ILE
1	C	201	THR
1	C	214	GLU
1	C	220	LEU
1	C	225	ARG
1	C	253	THR
1	C	270	LEU
1	C	277	GLU
1	C	315	ILE
1	D	8	ILE
1	D	21	ARG
1	D	24	VAL
1	D	42	GLU
1	D	48	LYS
1	D	62	SER
1	D	118	LEU
1	D	136	THR
1	D	140	LEU
1	D	153	LYS
1	D	169	ILE
1	D	190	LEU
1	D	206	LEU
1	D	220	LEU
1	D	223	LYS
1	D	225	ARG
1	D	249	VAL
1	D	271	SER
1	D	284	LYS
1	E	17	LYS
1	E	19	GLN
1	E	24	VAL
1	E	29	THR
1	E	47	VAL

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Mol	Chain	Res	Type
1	E	66	ILE
1	E	95	LEU
1	E	101	HIS
1	E	118	LEU
1	E	127	THR
1	E	158	ASP
1	E	177	ILE
1	E	206	LEU
1	E	217	SER
1	E	223	LYS
1	E	266	LYS
1	E	285	THR
1	E	303	CYS
1	E	315	ILE
1	E	319	ASN
1	F	4	LYS
1	F	10	ILE
1	F	24	VAL
1	F	31	LEU
1	F	39	LYS
1	F	58	ILE
1	F	65	GLN
1	F	79	GLN
1	F	101	HIS
1	F	121	ILE
1	F	166	THR
1	F	196	LYS
1	F	201	THR
1	F	213	GLU
1	F	225	ARG
1	F	290	THR
1	F	300	THR
1	F	303	CYS
1	F	309	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	HIS
1	B	90	ASN
1	B	126	HIS
1	C	79	GLN

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Mol	Chain	Res	Type
1	D	60	ASN
1	D	79	GLN
1	D	311	ASN
1	E	19	GLN
1	E	69	ASN
1	E	115	HIS
1	E	187	HIS
1	F	60	ASN
1	F	79	GLN
1	F	126	HIS
1	F	139	ASN
1	F	141	HIS
1	F	143	GLN
1	F	319	ASN

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](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 for Mogul analysis.

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	UL0	A	1003	-	41,43,43	1.40	3 (7%)	44,62,62	1.23	6 (13%)
3	UL0	D	1003	-	41,43,43	1.51	3 (7%)	44,62,62	1.24	3 (6%)
3	UL0	C	1003	-	41,43,43	1.44	3 (7%)	44,62,62	1.02	4 (9%)
3	UL0	B	1003	-	41,43,43	1.56	4 (9%)	44,62,62	1.36	4 (9%)
3	UL0	F	1003	-	41,43,43	1.50	3 (7%)	44,62,62	1.34	5 (11%)
3	UL0	E	1003	-	41,43,43	1.57	3 (7%)	44,62,62	1.14	5 (11%)

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	UL0	A	1003	-	-	6/29/60/60	0/5/5/5
3	UL0	D	1003	-	-	3/29/60/60	0/5/5/5
3	UL0	C	1003	-	-	5/29/60/60	0/5/5/5
3	UL0	B	1003	-	-	5/29/60/60	0/5/5/5
3	UL0	F	1003	-	-	4/29/60/60	0/5/5/5
3	UL0	E	1003	-	-	3/29/60/60	0/5/5/5

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1003	UL0	C23-N3	7.43	1.58	1.47
3	D	1003	UL0	C23-N3	7.32	1.58	1.47
3	B	1003	UL0	C23-N3	6.81	1.57	1.47
3	C	1003	UL0	C23-N3	6.60	1.56	1.47
3	F	1003	UL0	C23-N3	6.43	1.56	1.47
3	A	1003	UL0	C23-N3	6.13	1.56	1.47
3	F	1003	UL0	C6-N3	5.37	1.55	1.47
3	E	1003	UL0	C6-N3	5.25	1.54	1.47
3	B	1003	UL0	C6-N3	5.17	1.54	1.47
3	A	1003	UL0	C6-N3	4.82	1.54	1.47
3	C	1003	UL0	C6-N3	4.72	1.54	1.47
3	D	1003	UL0	C24-N3	3.87	1.51	1.47
3	F	1003	UL0	C24-N3	3.81	1.51	1.47
3	A	1003	UL0	C24-N3	3.80	1.51	1.47
3	E	1003	UL0	C24-N3	3.78	1.51	1.47
3	D	1003	UL0	C6-N3	3.76	1.52	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1003	UL0	C24-N3	3.73	1.51	1.47
3	C	1003	UL0	C24-N3	3.63	1.51	1.47
3	B	1003	UL0	C6-C5	-2.02	1.50	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	UL0	C6-C5-C4	-7.02	104.92	114.96
3	D	1003	UL0	C6-C5-C4	-6.02	106.36	114.96
3	F	1003	UL0	C6-C5-C4	-5.98	106.41	114.96
3	A	1003	UL0	C6-C5-C4	-3.96	109.31	114.96
3	F	1003	UL0	C23-C7-C5	3.65	108.51	103.36
3	C	1003	UL0	C6-C5-C4	-3.53	109.92	114.96
3	E	1003	UL0	C6-C5-C4	-3.38	110.13	114.96
3	E	1003	UL0	C6-C5-C7	3.02	108.86	103.42
3	E	1003	UL0	C10-C11-C12	-3.01	108.29	113.53
3	A	1003	UL0	C14-C13-C12	2.71	133.92	125.27
3	A	1003	UL0	C14-C13-C16	-2.65	122.64	126.56
3	B	1003	UL0	C10-C11-C12	-2.50	109.16	113.53
3	E	1003	UL0	C23-C7-C5	2.50	106.89	103.36
3	B	1003	UL0	C14-C13-C12	2.36	132.81	125.27
3	A	1003	UL0	C7-C8-N	2.31	117.53	114.05
3	B	1003	UL0	C12-N2-N1	-2.26	111.39	113.81
3	C	1003	UL0	C21-C11-C12	2.25	117.46	113.53
3	A	1003	UL0	C17-C16-N1	2.21	123.44	119.65
3	E	1003	UL0	C23-N3-C6	2.16	107.27	104.12
3	C	1003	UL0	C12-N2-N1	-2.13	111.53	113.81
3	F	1003	UL0	C12-N2-N1	-2.13	111.53	113.81
3	D	1003	UL0	C23-C7-C5	2.10	106.33	103.36
3	F	1003	UL0	C14-C13-C12	2.10	131.98	125.27
3	A	1003	UL0	C6-C5-C7	2.09	107.20	103.42
3	F	1003	UL0	C23-N3-C6	2.08	107.15	104.12
3	C	1003	UL0	C23-C7-C5	2.07	106.28	103.36
3	D	1003	UL0	C22-N-C8	-2.01	105.79	111.35

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	UL0	C25-C24-N3-C6
3	A	1003	UL0	C7-C8-N-C9
3	B	1003	UL0	C25-C24-N3-C6

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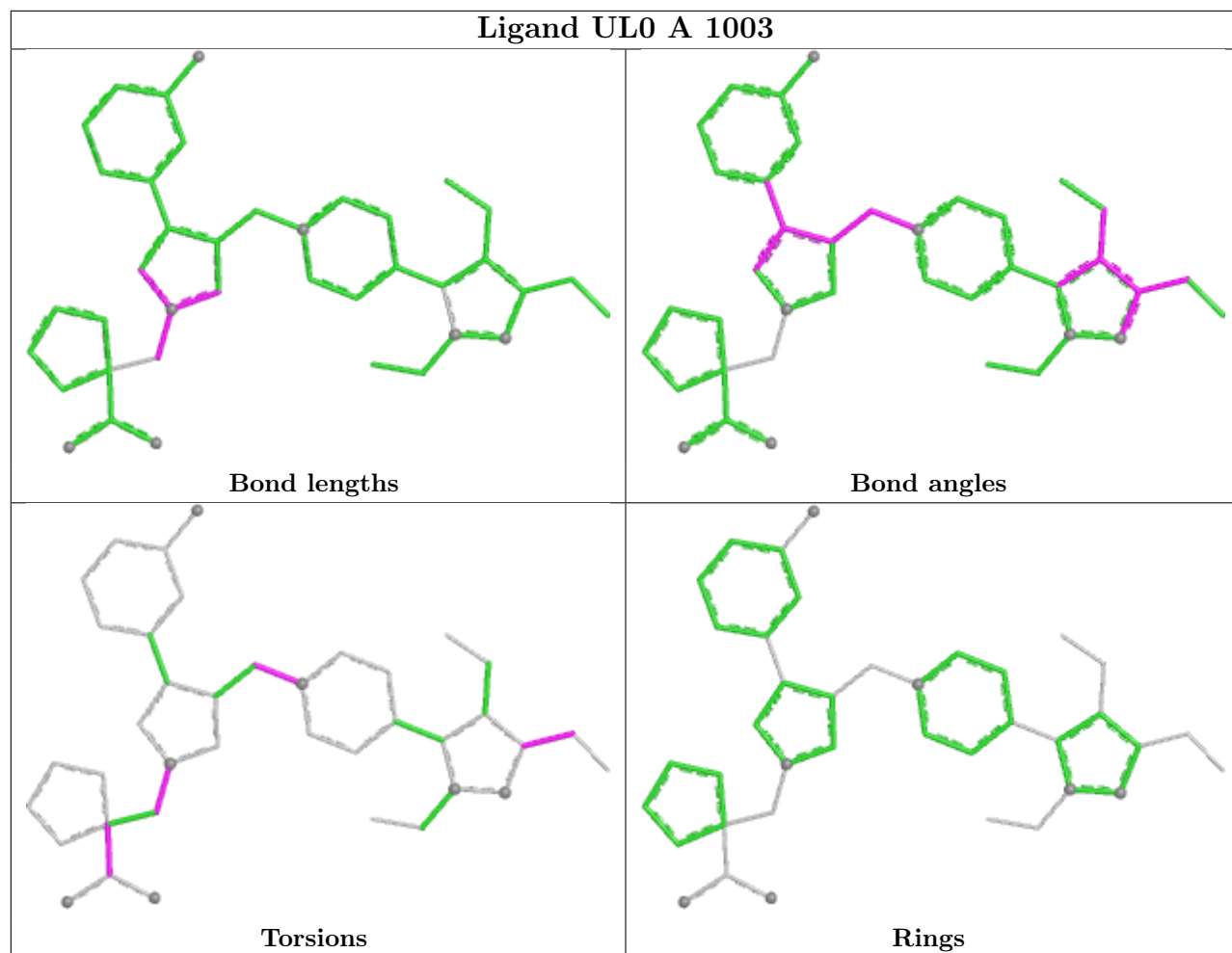
Mol	Chain	Res	Type	Atoms
3	B	1003	UL0	N3-C24-C25-C30
3	C	1003	UL0	C25-C24-N3-C6
3	D	1003	UL0	C25-C24-N3-C6
3	E	1003	UL0	C25-C24-N3-C6
3	E	1003	UL0	C27-C25-C26-O
3	F	1003	UL0	C25-C24-N3-C6
3	A	1003	UL0	C24-C25-C26-O1
3	A	1003	UL0	C24-C25-C26-O
3	C	1003	UL0	C27-C25-C26-O1
3	E	1003	UL0	C27-C25-C26-O1
3	F	1003	UL0	C27-C25-C26-O
3	C	1003	UL0	C27-C25-C26-O
3	F	1003	UL0	C27-C25-C26-O1
3	D	1003	UL0	C27-C25-C26-O1
3	D	1003	UL0	C27-C25-C26-O
3	B	1003	UL0	N1-C16-C17-C18
3	B	1003	UL0	N3-C24-C25-C27
3	A	1003	UL0	C13-C16-C17-C18
3	B	1003	UL0	C13-C16-C17-C18
3	C	1003	UL0	C12-C13-C14-C15
3	C	1003	UL0	C30-C25-C26-O1
3	A	1003	UL0	N1-C16-C17-C18
3	F	1003	UL0	N1-C16-C17-C18

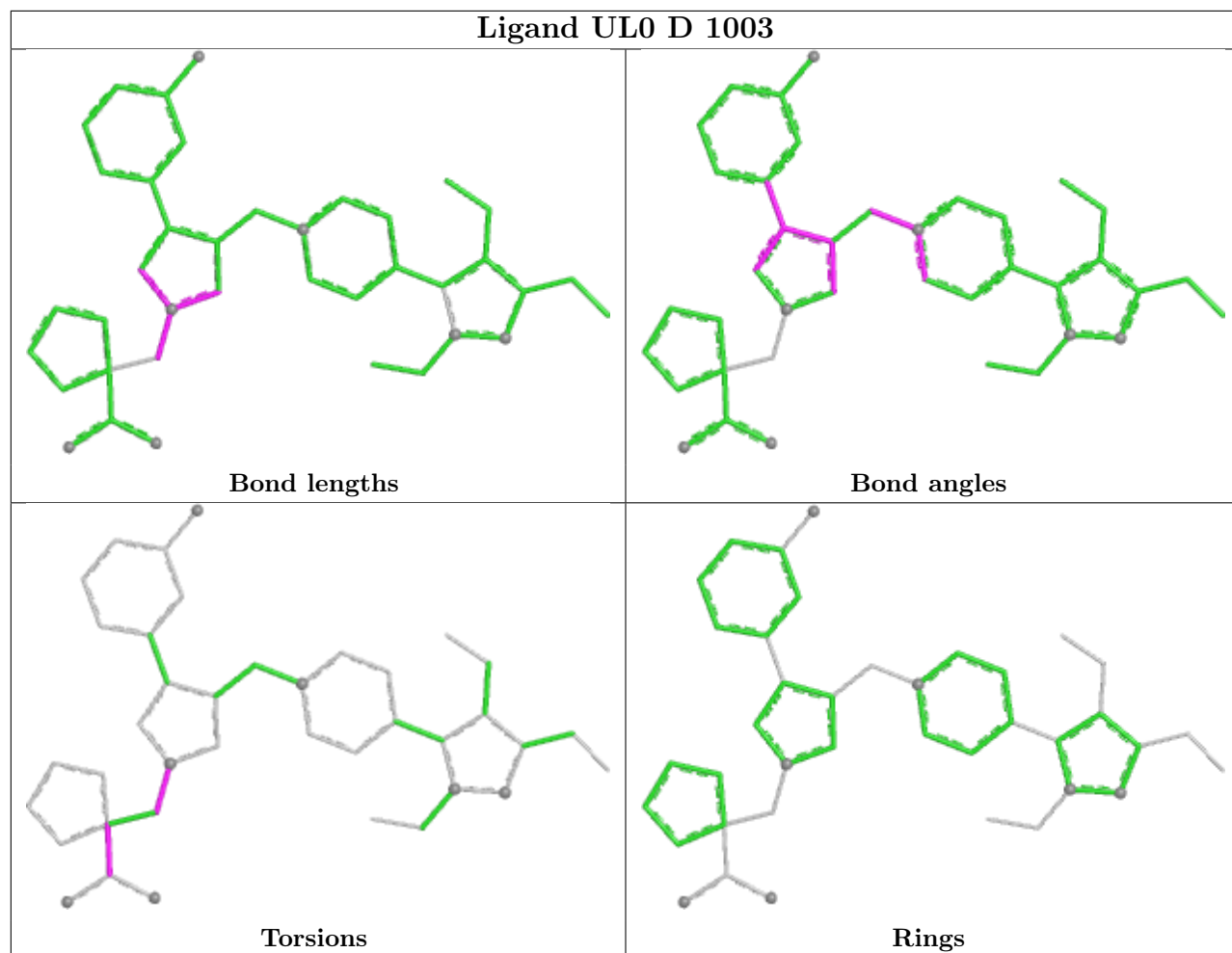
There are no ring outliers.

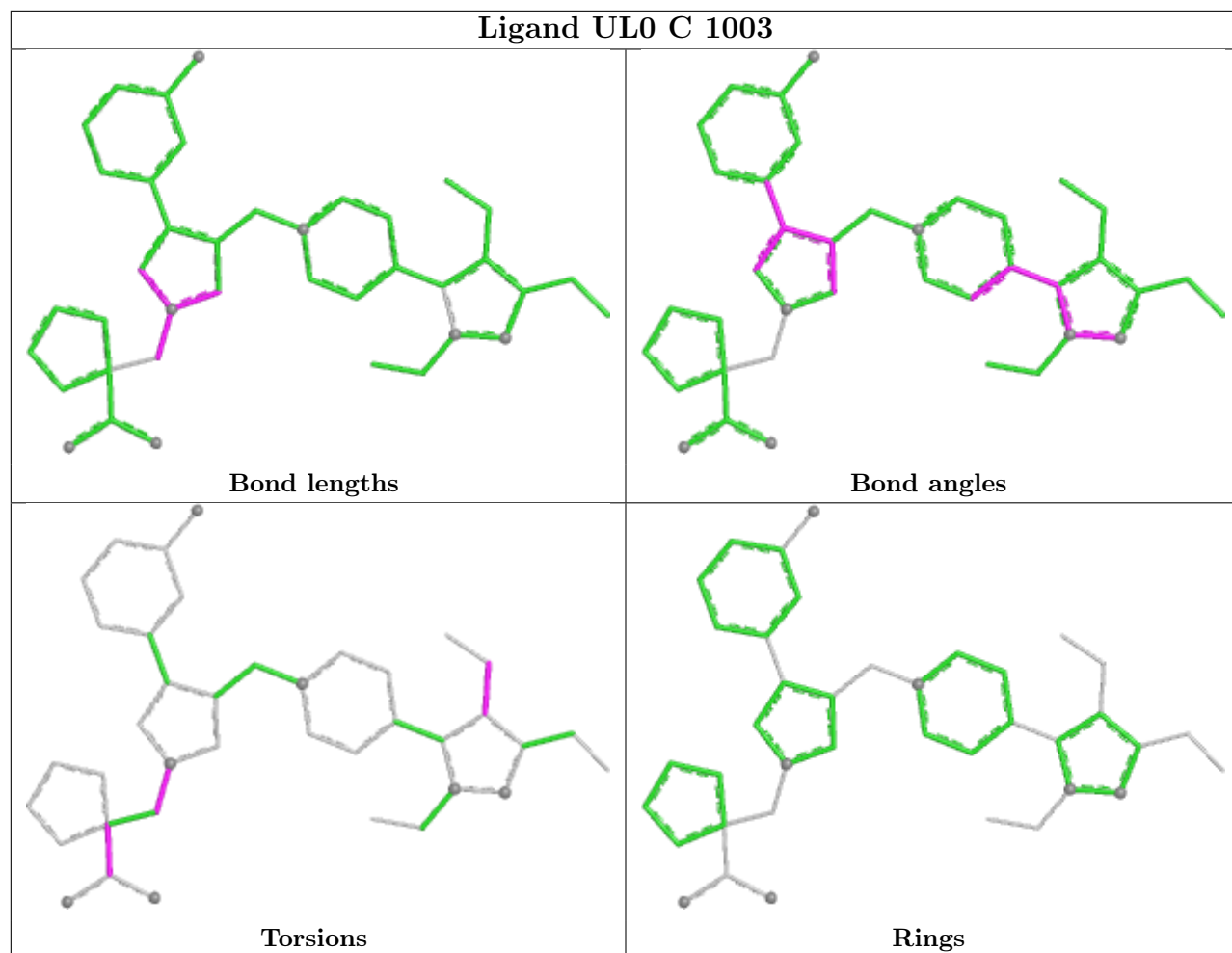
1 monomer is involved in 1 short contact:

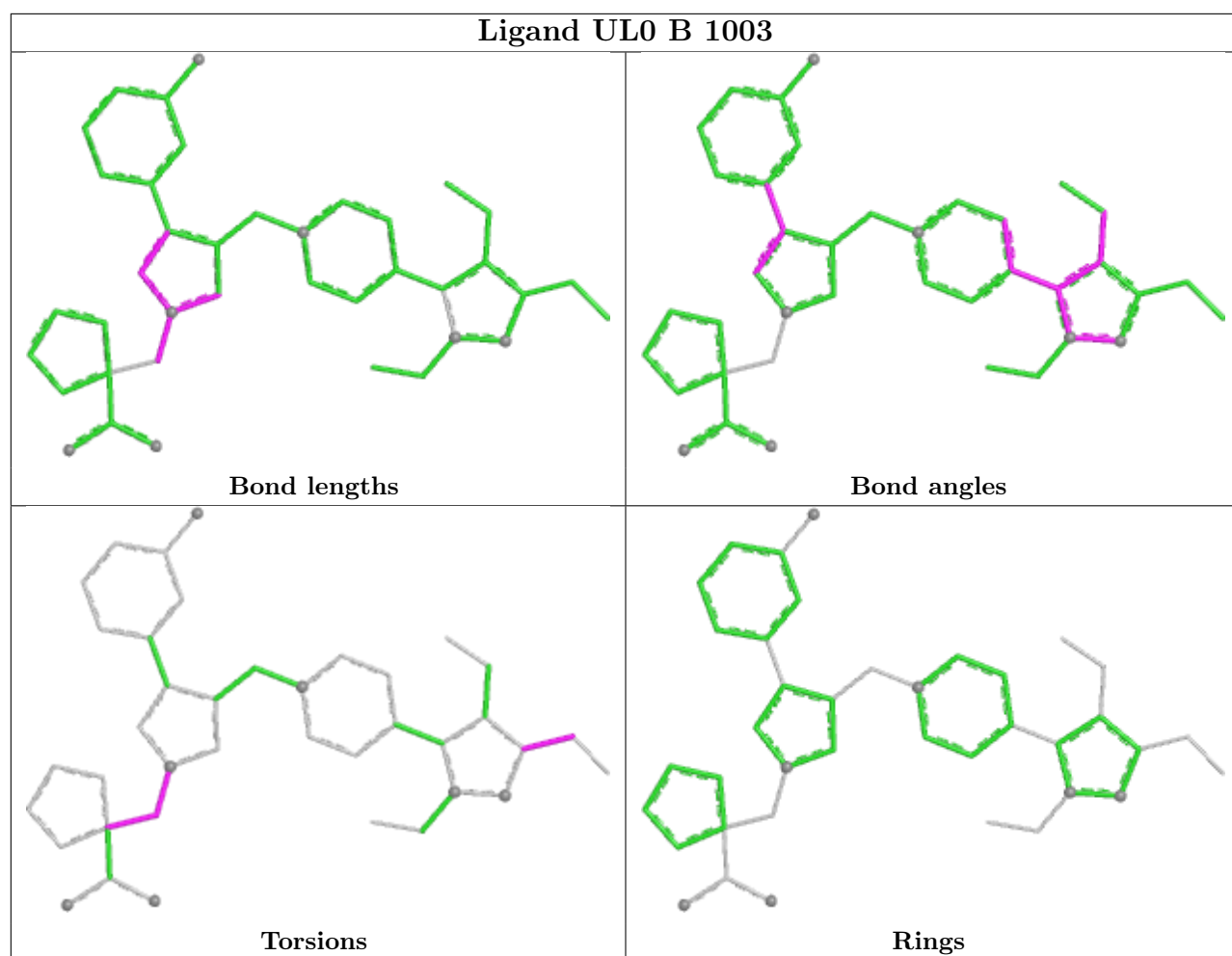
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1003	UL0	1	0

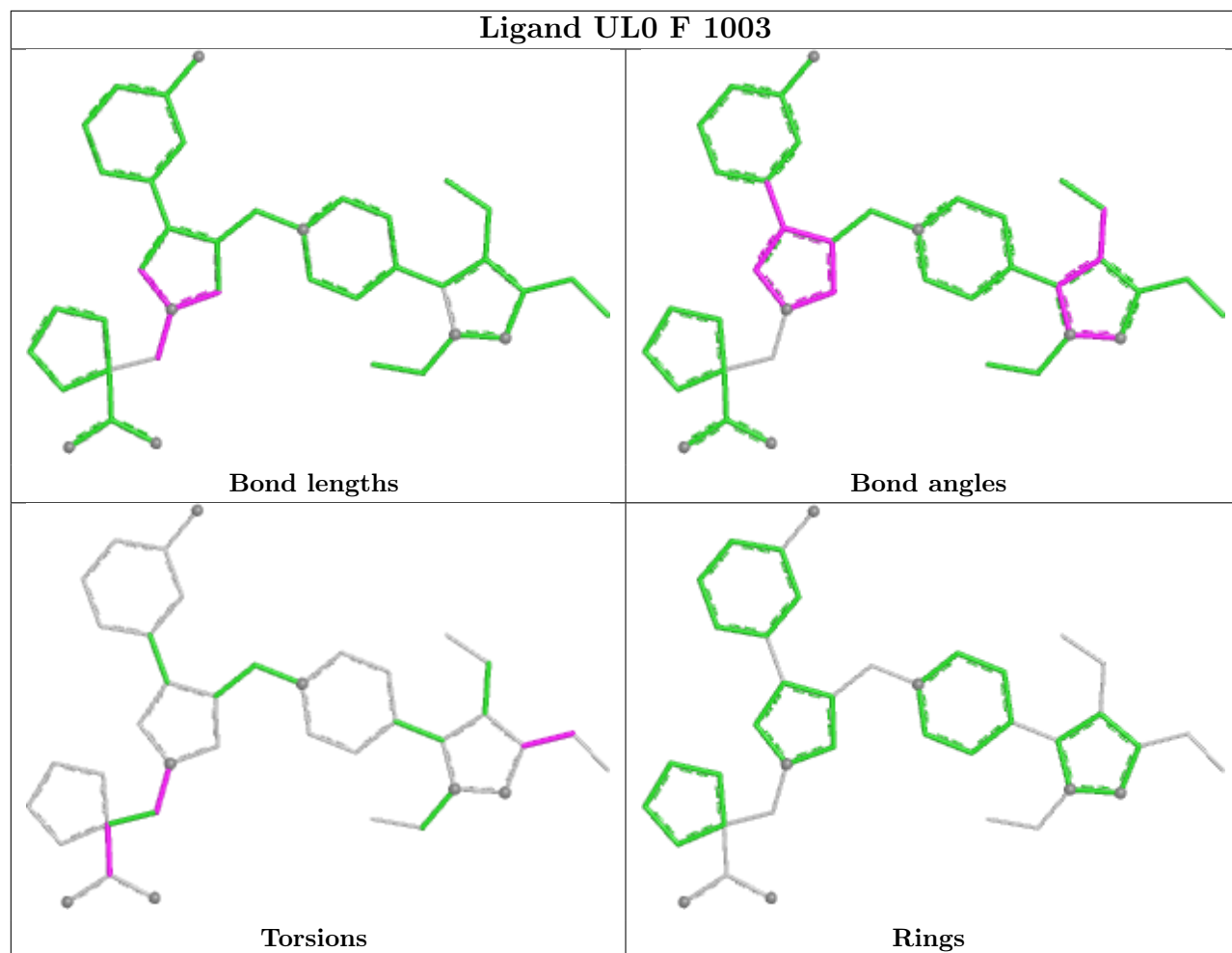
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

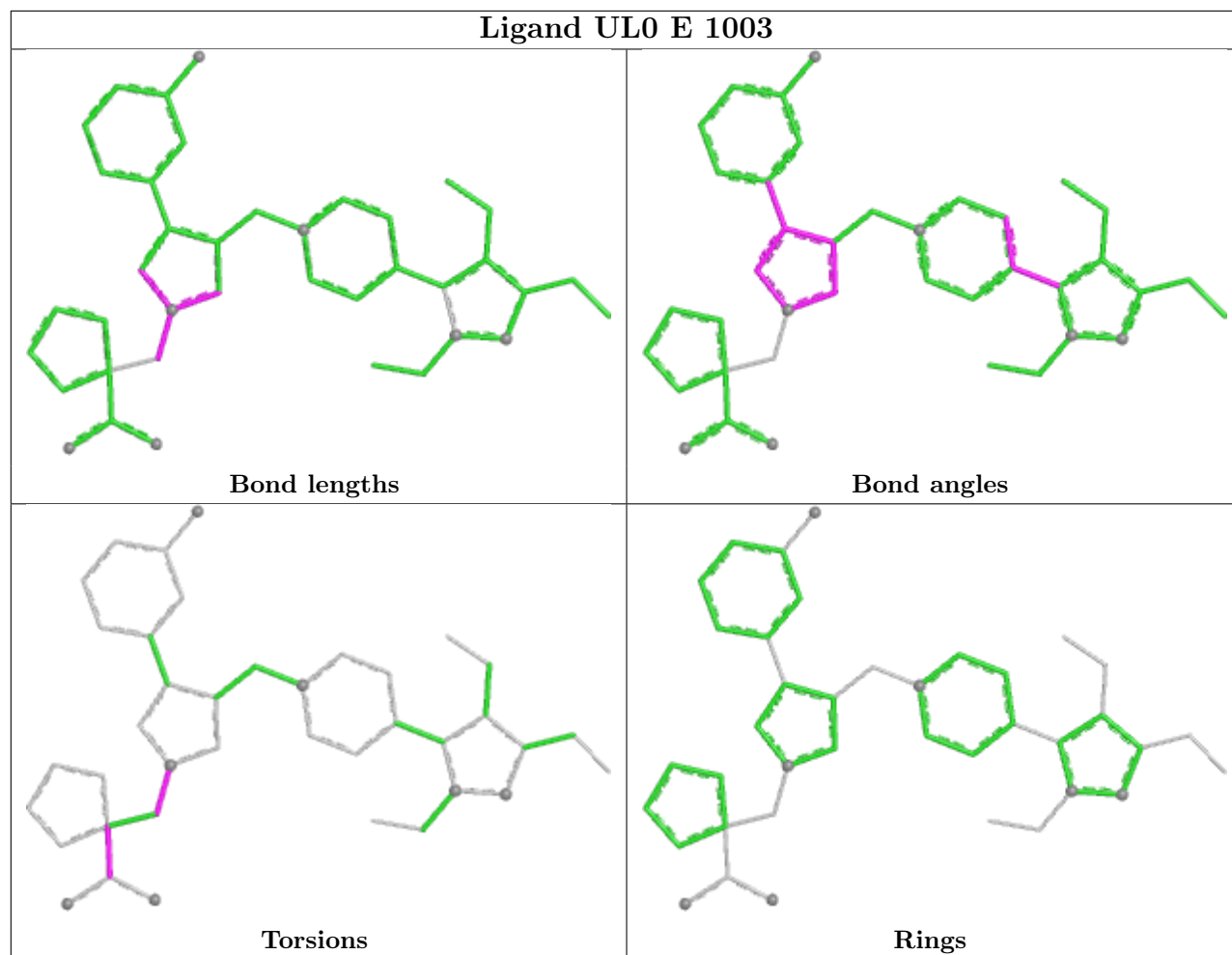












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	317/322 (98%)	-1.59	0 100 100	11, 21, 35, 42	0
1	B	317/322 (98%)	-1.57	0 100 100	8, 21, 30, 44	0
1	C	317/322 (98%)	-1.60	0 100 100	10, 21, 33, 43	0
1	D	317/322 (98%)	-1.53	0 100 100	9, 22, 30, 38	0
1	E	317/322 (98%)	-1.47	0 100 100	10, 27, 41, 51	0
1	F	317/322 (98%)	-1.47	0 100 100	11, 25, 41, 47	0
All	All	1902/1932 (98%)	-1.54	0 100 100	8, 22, 37, 51	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MN	A	1002	1/1	0.99	0.02	19,19,19,19	0

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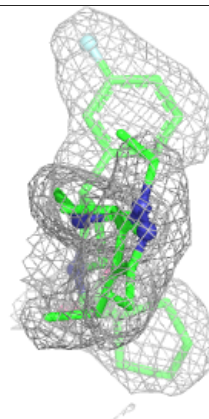
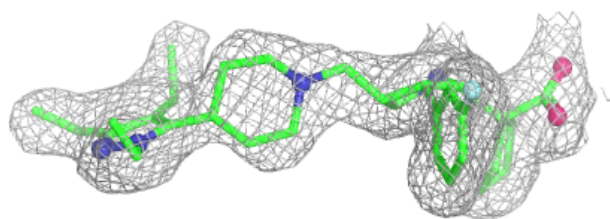
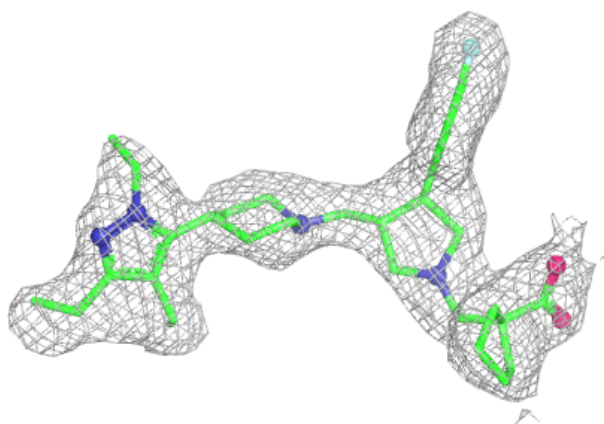
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	UL0	A	1003	39/39	0.99	0.03	14,16,19,19	0
3	UL0	B	1003	39/39	0.99	0.04	18,22,25,25	0
3	UL0	C	1003	39/39	0.99	0.03	17,19,24,25	0
3	UL0	D	1003	39/39	0.99	0.03	13,16,18,18	0
3	UL0	E	1003	39/39	0.99	0.04	24,27,28,28	0
3	UL0	F	1003	39/39	0.99	0.03	16,23,25,26	0
2	MN	D	1002	1/1	1.00	0.02	35,35,35,35	0
2	MN	E	1001	1/1	1.00	0.01	24,24,24,24	0
2	MN	E	1002	1/1	1.00	0.01	22,22,22,22	0
2	MN	F	1001	1/1	1.00	0.02	38,38,38,38	0
2	MN	F	1002	1/1	1.00	0.01	28,28,28,28	0
2	MN	A	1001	1/1	1.00	0.01	15,15,15,15	0
2	MN	B	1001	1/1	1.00	0.01	21,21,21,21	0
2	MN	B	1002	1/1	1.00	0.01	16,16,16,16	0
2	MN	C	1001	1/1	1.00	0.03	26,26,26,26	0
2	MN	C	1002	1/1	1.00	0.01	26,26,26,26	0
2	MN	D	1001	1/1	1.00	0.03	40,40,40,40	0

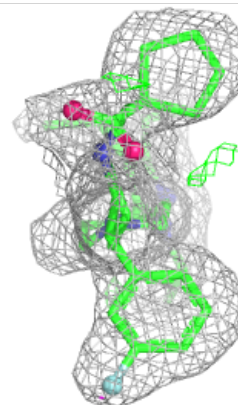
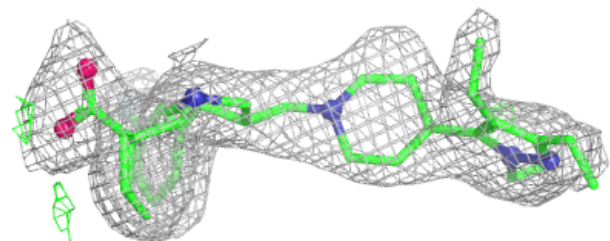
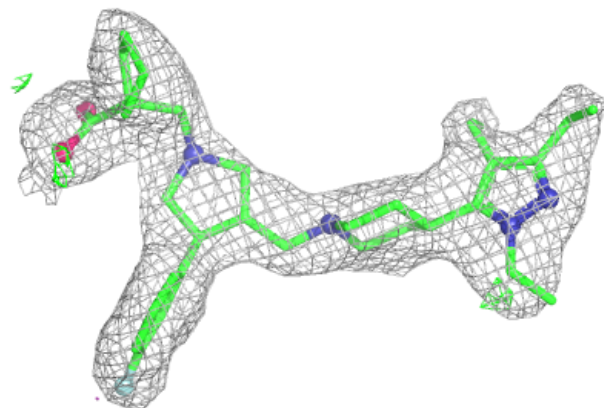
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around UL0 A 1003:

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

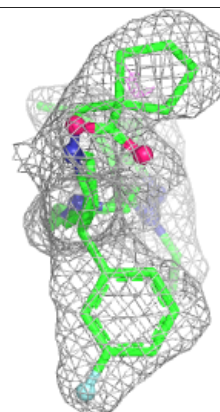
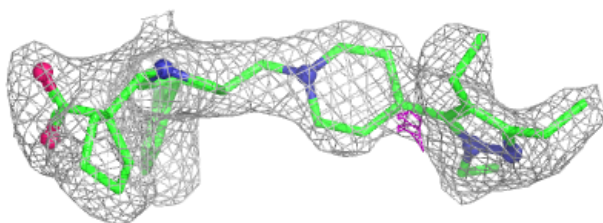
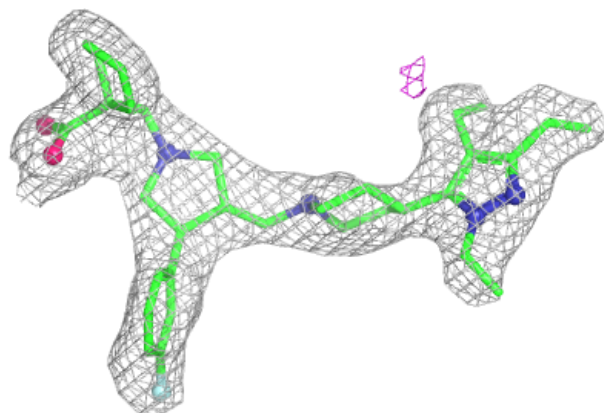
**Electron density around UL0 B 1003:**

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

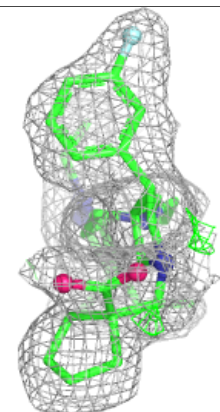
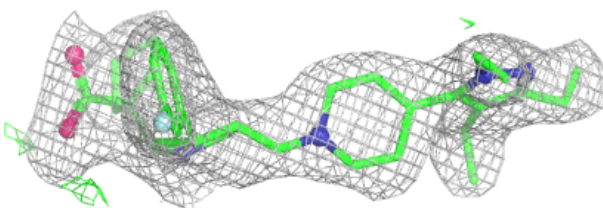
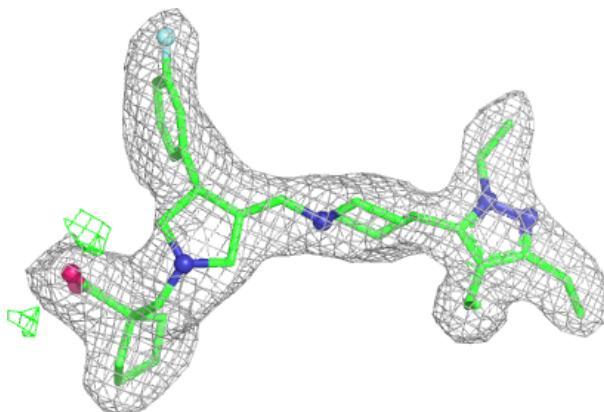


Electron density around UL0 C 1003:

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

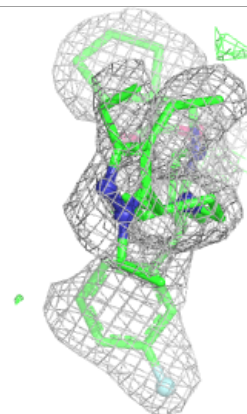
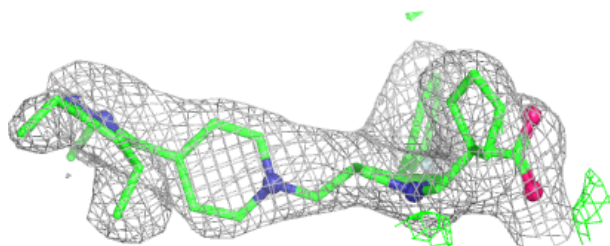
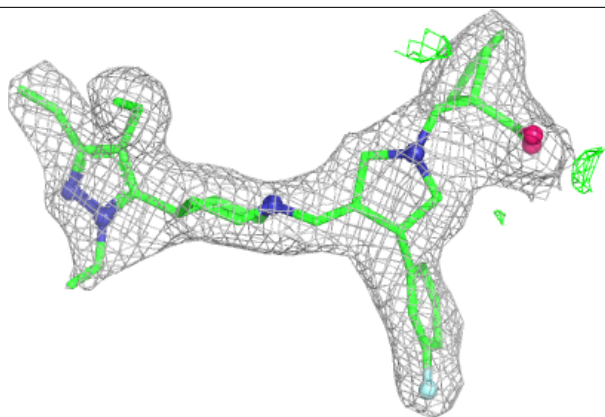
**Electron density around UL0 D 1003:**

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

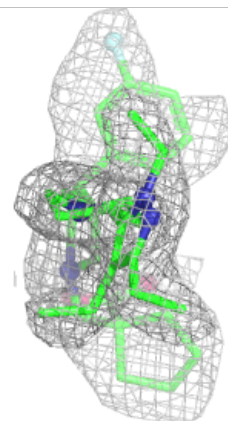
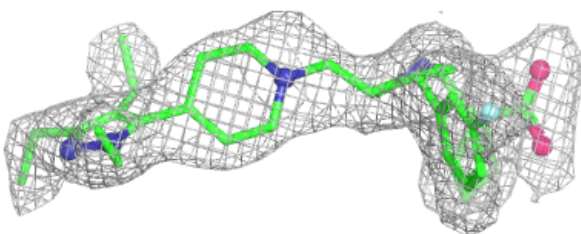
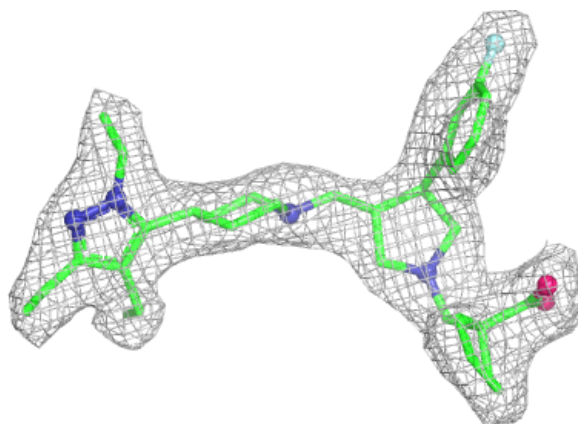


Electron density around UL0 E 1003:

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

**Electron density around UL0 F 1003:**

$2mF_o-DF_c$ (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.