



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 6, 2022 – 04:05 PM EST

PDB ID : 7T0T
Title : Crystal structure of the BCL6 BTB domain in complex with OICR-10562
Authors : Kuntz, D.A.; Prive, G.G.
Deposited on : 2021-11-30
Resolution : 2.00 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.31.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

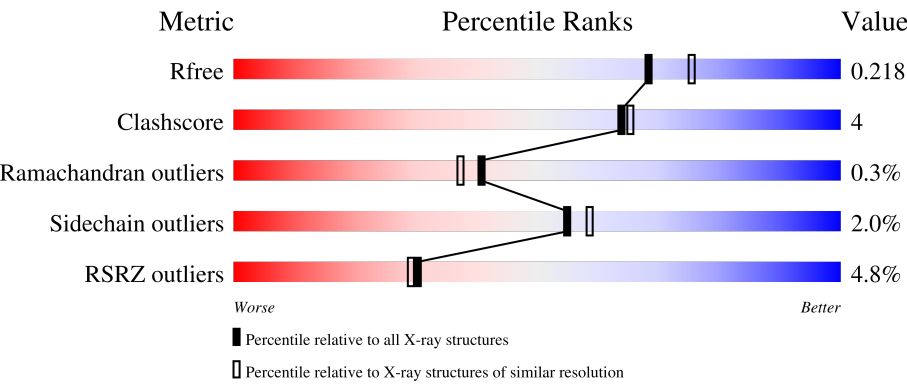
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	127	<div><div>2%</div><div></div><div>86%</div><div>11%</div><div></div></div>
1	B	127	<div><div>3%</div><div></div><div>86%</div><div>10%</div><div></div></div>
1	C	127	<div><div>5%</div><div></div><div>88%</div><div>9%</div><div></div></div>
1	D	127	<div><div>8%</div><div></div><div>87%</div><div>8%</div><div>5%</div></div>
1	E	127	<div><div>6%</div><div></div><div>77%</div><div>17%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	127	<div><div></div><div>4%</div><div></div><div>85%</div><div></div><div>10%</div><div></div><div></div></div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12809 atoms, of which 6125 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 Isoform 2 of B-cell lymphoma 6 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	123	Total	C	H	N	O	S	0	5	0
			2031	639	1024	176	184	8			
1	B	122	Total	C	H	N	O	S	0	10	0
			2058	643	1040	182	185	8			
1	C	123	Total	C	H	N	O	S	0	8	0
			2053	652	1022	185	186	8			
1	D	121	Total	C	H	N	O	S	0	10	0
			2008	636	1003	177	184	8			
1	E	122	Total	C	H	N	O	S	0	5	0
			2005	630	1013	176	178	8			
1	F	122	Total	C	H	N	O	S	0	4	0
			1998	627	1011	174	178	8			

There are 30 discrepancies between the modelled and reference sequences:

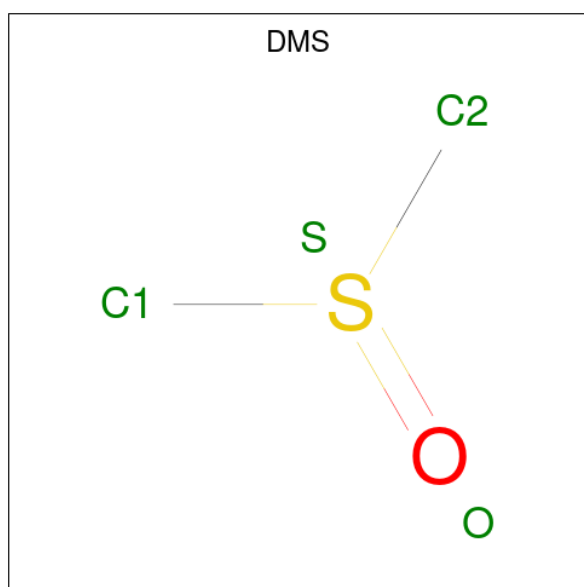
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P41182
A	4	SER	-	expression tag	UNP P41182
A	8	GLN	CYS	engineered mutation	UNP P41182
A	67	ARG	CYS	engineered mutation	UNP P41182
A	84	ASN	CYS	engineered mutation	UNP P41182
B	3	GLY	-	expression tag	UNP P41182
B	4	SER	-	expression tag	UNP P41182
B	8	GLN	CYS	engineered mutation	UNP P41182
B	67	ARG	CYS	engineered mutation	UNP P41182
B	84	ASN	CYS	engineered mutation	UNP P41182
C	3	GLY	-	expression tag	UNP P41182
C	4	SER	-	expression tag	UNP P41182
C	8	GLN	CYS	engineered mutation	UNP P41182
C	67	ARG	CYS	engineered mutation	UNP P41182
C	84	ASN	CYS	engineered mutation	UNP P41182
D	3	GLY	-	expression tag	UNP P41182
D	4	SER	-	expression tag	UNP P41182

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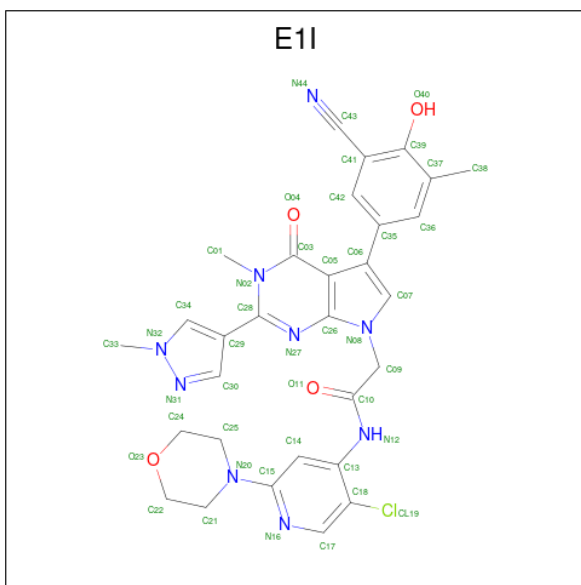
Chain	Residue	Modelled	Actual	Comment	Reference
D	8	GLN	CYS	engineered mutation	UNP P41182
D	67	ARG	CYS	engineered mutation	UNP P41182
D	84	ASN	CYS	engineered mutation	UNP P41182
E	3	GLY	-	expression tag	UNP P41182
E	4	SER	-	expression tag	UNP P41182
E	8	GLN	CYS	engineered mutation	UNP P41182
E	67	ARG	CYS	engineered mutation	UNP P41182
E	84	ASN	CYS	engineered mutation	UNP P41182
F	3	GLY	-	expression tag	UNP P41182
F	4	SER	-	expression tag	UNP P41182
F	8	GLN	CYS	engineered mutation	UNP P41182
F	67	ARG	CYS	engineered mutation	UNP P41182
F	84	ASN	CYS	engineered mutation	UNP P41182

- Molecule 2 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
2	E	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 3 is N-[5-chloro-2-(morpholin-4-yl)pyridin-4-yl]-2-[5-(3-cyano-4-hydroxy-5-methyl phenyl)-3-methyl-2-(1-methyl-1H-pyrazol-4-yl)-4-oxo-3,4-dihydro-7H-pyrrolo[2,3-d]pyrimidin-7-yl]acetamide (three-letter code: E1I) (formula: C₃₀H₂₈ClN₉O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		
3	B	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		
3	C	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		
3	D	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		
3	E	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		
3	F	1	Total	C	Cl	N	O	0	0
			44	30	1	9	4		

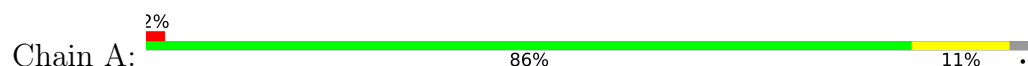
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	70	Total	O	0	2
			72	72		
4	B	65	Total	O	0	1
			66	66		
4	C	57	Total	O	0	0
			57	57		
4	D	61	Total	O	0	0
			61	61		
4	E	60	Total	O	0	1
			61	61		
4	F	55	Total	O	0	0
			55	55		

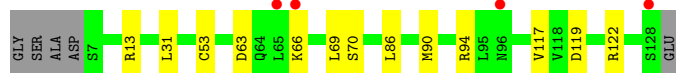
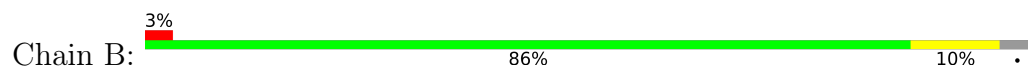
3 Residue-property plots [i](#)

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

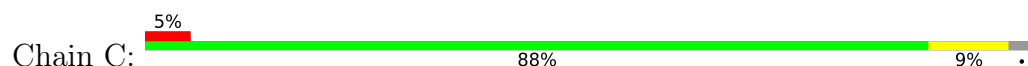
- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



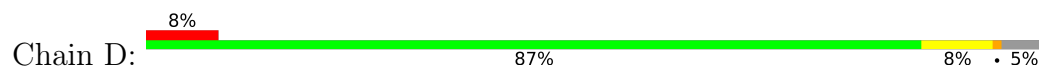
- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



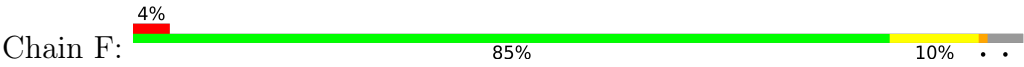
- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



- Molecule 1: Isoform 2 of B-cell lymphoma 6 protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	62.59Å 102.55Å 65.03Å 90.00° 115.48° 90.00°	Depositor
Resolution (Å)	32.36 – 2.00 32.36 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (32.36-2.00) 99.7 (32.36-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.181 , 0.219 0.181 , 0.218	Depositor DCC
R_{free} test set	2544 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12809	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.59% 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: E1I, DMS

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	0.34	0/1037	0.55	0/1399
1	B	0.35	0/1069	0.56	0/1443
1	C	0.38	0/1067	0.55	0/1437
1	D	0.34	0/1053	0.55	0/1422
1	E	0.36	0/1020	0.61	1/1379 (0.1%)
1	F	0.36	0/1016	0.54	0/1370
All	All	0.36	0/6262	0.56	1/8450 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	24	ARG	NE-CZ-NH2	-5.96	117.32	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	43	PHE	Mainchain
1	C	44[B]	ARG	Mainchain

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	1007	1024	1026	9	0
1	B	1018	1040	1020	7	0
1	C	1031	1022	1042	6	0
1	D	1005	1003	1001	6	0
1	E	992	1013	1006	20	0
1	F	987	1011	1008	10	0
2	A	4	6	6	0	0
2	E	4	6	6	0	0
3	A	44	0	0	0	0
3	B	44	0	0	0	0
3	C	44	0	0	0	0
3	D	44	0	0	0	0
3	E	44	0	0	1	0
3	F	44	0	0	2	0
4	A	72	0	0	0	0
4	B	66	0	0	0	0
4	C	57	0	0	0	0
4	D	61	0	0	1	0
4	E	61	0	0	1	0
4	F	55	0	0	0	0
All	All	6684	6125	6115	53	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 4.

All (53) 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:60:ILE:HA	1:E:65:LEU:HD11	1.73	0.70
1:F:38:VAL:HG22	1:F:74:LEU:HD12	1.76	0.68
1:E:97:LEU:HD22	1:E:102:ILE:HD13	1.82	0.60
1:A:63:ASP:OD2	1:A:66:LYS:HG2	2.03	0.59
1:A:8:GLN:OE1	1:B:94:ARG:NE	2.35	0.59
1:C:97:LEU:HD11	1:C:102:ILE:HD12	1.88	0.54
1:E:65:LEU:HD12	1:E:66:LYS:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:ILE:HG23	1:F:103:MET:H	1.72	0.54
1:D:69:LEU:HB2	1:D:72:ILE:HD11	1.91	0.53
1:D:92:THR:O	1:D:93:SER:HB2	2.09	0.52
1:F:102:ILE:HG23	1:F:103:MET:N	2.24	0.52
1:F:35:VAL:HG22	1:F:44:ARG:NH1	2.25	0.52
1:B:53:CYS:CB	1:B:90:MET:HG2	2.39	0.51
1:F:38:VAL:HG13	1:F:78:ILE:HG22	1.93	0.51
1:E:63:ASP:HB2	1:E:65:LEU:HD23	1.92	0.51
1:E:93:SER:OG	1:F:10:GLN:NE2	2.41	0.50
1:A:47:LYS:O	1:A:51:MET:HG3	2.12	0.50
1:C:98:ARG:HH12	1:D:5:ALA:HB2	1.77	0.50
1:F:58:TYR:CE1	1:F:62:THR:HG21	2.48	0.48
1:E:24:ARG:NE	1:E:24:ARG:HA	2.28	0.48
1:A:119:ASP:OD1	1:A:122:ARG:NH1	2.46	0.48
1:C:75:ASP:HB3	1:C:77:GLU:OE1	2.13	0.48
1:E:63:ASP:HB2	1:E:65:LEU:CD2	2.44	0.48
1:E:65:LEU:O	1:E:67:ARG:N	2.47	0.48
1:E:26:ARG:HD3	1:E:91:TYR:CZ	2.49	0.47
1:A:58:TYR:O	1:A:62:THR:HG23	2.13	0.47
1:E:102:ILE:HG23	1:E:103:MET:CE	2.44	0.47
1:E:117:VAL:HG23	3:E:201:E1I:N44	2.29	0.47
1:E:24:ARG:O	1:E:28:ARG:HG2	2.15	0.46
1:B:119:ASP:OD1	1:B:122:ARG:NH2	2.48	0.46
1:C:97:LEU:HD11	1:C:102:ILE:CD1	2.46	0.46
1:D:44[B]:ARG:NH1	4:D:301:HOH:O	2.38	0.46
1:F:86:LEU:HD21	1:F:117:VAL:HG11	1.99	0.45
1:E:47:LYS:O	1:E:51:MET:HG3	2.17	0.45
1:E:126:LYS:O	1:E:126:LYS:HD2	2.17	0.45
1:C:53:CYS:CB	1:C:90:MET:HG2	2.47	0.45
1:A:60:ILE:O	1:A:66:LYS:HB2	2.17	0.44
1:B:66:LYS:CB	1:B:69:LEU:HD12	2.47	0.44
1:E:86:LEU:HD21	1:E:117:VAL:HG11	1.99	0.44
1:B:86:LEU:HD11	1:B:117:VAL:HG11	1.99	0.44
1:E:24:ARG:HG2	3:F:201:E1I:N16	2.33	0.44
1:E:62:THR:O	1:E:67:ARG:NH1	2.51	0.44
1:C:53:CYS:HB3	1:C:90:MET:HG2	1.99	0.43
1:A:86:LEU:HD21	1:A:117:VAL:HG11	2.01	0.43
1:E:53:CYS:CB	1:E:90:MET:HG2	2.49	0.42
1:E:24:ARG:HD2	4:E:356[A]:HOH:O	2.18	0.42
1:F:38:VAL:HG11	1:F:80:PRO:HA	2.01	0.42
1:D:86:LEU:HD21	1:D:117:VAL:HG11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:117:VAL:HG23	3:F:201:EII:N44	2.34	0.42
1:A:67:ARG:HD3	1:B:31:LEU:HG	2.02	0.41
1:E:63:ASP:C	1:E:65:LEU:N	2.75	0.41
1:D:56:LEU:O	1:D:60:ILE:HG13	2.21	0.40
1:A:8:GLN:OE1	1:B:94:ARG:CG	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	126/127 (99%)	124 (98%)	2 (2%)	0	100	100
1	B	130/127 (102%)	128 (98%)	2 (2%)	0	100	100
1	C	129/127 (102%)	126 (98%)	3 (2%)	0	100	100
1	D	127/127 (100%)	123 (97%)	4 (3%)	0	100	100
1	E	125/127 (98%)	121 (97%)	2 (2%)	2 (2%)	9	4
1	F	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
All	All	761/762 (100%)	742 (98%)	17 (2%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	66	LYS
1	E	64	GLN

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	115/115 (100%)	114 (99%)	1 (1%)	78	83
1	B	118/115 (103%)	114 (97%)	4 (3%)	37	36
1	C	119/115 (104%)	117 (98%)	2 (2%)	60	65
1	D	116/115 (101%)	114 (98%)	2 (2%)	60	65
1	E	112/115 (97%)	108 (96%)	4 (4%)	35	34
1	F	113/115 (98%)	111 (98%)	2 (2%)	59	63
All	All	693/690 (100%)	678 (98%)	15 (2%)	55	55

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	B	13[A]	ARG
1	B	13[B]	ARG
1	B	63	ASP
1	B	70	SER
1	C	8	GLN
1	C	79	ASN
1	D	69	LEU
1	D	96	ASN
1	E	13	ARG
1	E	94[A]	ARG
1	E	94[B]	ARG
1	E	103	MET
1	F	64	GLN
1	F	103	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	B	68	ASN
1	D	96	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	E1I	E	201	-	43,49,49	2.87	13 (30%)	51,72,72	2.42	15 (29%)
3	E1I	F	201	-	43,49,49	2.93	14 (32%)	51,72,72	2.23	16 (31%)
2	DMS	E	202	-	3,3,3	0.64	0	3,3,3	0.64	0
2	DMS	A	201	-	3,3,3	0.69	0	3,3,3	0.44	0
3	E1I	B	201	-	43,49,49	2.96	14 (32%)	51,72,72	2.06	17 (33%)
3	E1I	D	201	-	43,49,49	2.92	16 (37%)	51,72,72	2.21	17 (33%)
3	E1I	A	202	-	43,49,49	2.93	13 (30%)	51,72,72	2.09	14 (27%)
3	E1I	C	201	-	43,49,49	2.88	13 (30%)	51,72,72	2.05	14 (27%)

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	E1I	E	201	-	-	4/18/30/30	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	E1I	F	201	-	-	1/18/30/30	0/6/6/6
3	E1I	B	201	-	-	0/18/30/30	0/6/6/6
3	E1I	D	201	-	-	2/18/30/30	0/6/6/6
3	E1I	A	202	-	-	1/18/30/30	0/6/6/6
3	E1I	C	201	-	-	0/18/30/30	0/6/6/6

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	E1I	C28-N27	11.09	1.46	1.29
3	A	202	E1I	C28-N27	11.07	1.46	1.29
3	D	201	E1I	C28-N27	10.94	1.45	1.29
3	E	201	E1I	C28-N27	10.39	1.45	1.29
3	F	201	E1I	C28-N27	10.29	1.44	1.29
3	C	201	E1I	C28-N27	10.18	1.44	1.29
3	F	201	E1I	C25-N20	7.64	1.58	1.46
3	E	201	E1I	C25-N20	7.28	1.58	1.46
3	D	201	E1I	C25-N20	7.17	1.58	1.46
3	C	201	E1I	C25-N20	7.14	1.57	1.46
3	A	202	E1I	C25-N20	7.11	1.57	1.46
3	B	201	E1I	C25-N20	6.97	1.57	1.46
3	C	201	E1I	C10-N12	6.26	1.49	1.35
3	D	201	E1I	C10-N12	5.76	1.48	1.35
3	F	201	E1I	C10-N12	5.74	1.48	1.35
3	B	201	E1I	C10-N12	5.73	1.48	1.35
3	A	202	E1I	C10-N12	5.58	1.48	1.35
3	E	201	E1I	C10-N12	5.17	1.47	1.35
3	F	201	E1I	C41-C43	5.06	1.52	1.44
3	A	202	E1I	C41-C43	4.95	1.51	1.44
3	F	201	E1I	C15-N20	4.95	1.47	1.37
3	D	201	E1I	C41-C43	4.90	1.51	1.44
3	E	201	E1I	C41-C43	4.89	1.51	1.44
3	E	201	E1I	C15-N20	4.67	1.47	1.37
3	B	201	E1I	C41-C43	4.67	1.51	1.44
3	A	202	E1I	C15-N20	4.56	1.46	1.37
3	B	201	E1I	C15-N20	4.55	1.46	1.37
3	D	201	E1I	C15-N20	4.53	1.46	1.37
3	C	201	E1I	C15-N20	4.53	1.46	1.37
3	B	201	E1I	C06-C35	-4.50	1.41	1.49
3	E	201	E1I	C06-C35	-4.44	1.41	1.49
3	D	201	E1I	C06-C35	-4.43	1.41	1.49
3	C	201	E1I	C06-C35	-4.38	1.41	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	E1I	C06-C35	-4.30	1.41	1.49
3	C	201	E1I	C41-C43	4.23	1.50	1.44
3	F	201	E1I	C06-C35	-4.11	1.42	1.49
3	C	201	E1I	C26-N27	4.10	1.47	1.37
3	C	201	E1I	C29-C28	4.02	1.54	1.47
3	E	201	E1I	C29-C28	4.00	1.54	1.47
3	B	201	E1I	C29-C28	3.95	1.54	1.47
3	D	201	E1I	C29-C28	3.90	1.54	1.47
3	A	202	E1I	C29-C28	3.89	1.54	1.47
3	B	201	E1I	C07-N08	-3.89	1.33	1.38
3	E	201	E1I	C07-N08	-3.82	1.33	1.38
3	F	201	E1I	C29-C28	3.82	1.54	1.47
3	A	202	E1I	C07-N08	-3.81	1.33	1.38
3	F	201	E1I	C26-N27	3.71	1.46	1.37
3	D	201	E1I	C07-N08	-3.54	1.34	1.38
3	B	201	E1I	C26-N27	3.52	1.45	1.37
3	B	201	E1I	C13-N12	3.47	1.48	1.41
3	C	201	E1I	C07-N08	-3.46	1.34	1.38
3	D	201	E1I	C26-N27	3.45	1.45	1.37
3	F	201	E1I	C07-N08	-3.45	1.34	1.38
3	E	201	E1I	C13-N12	3.39	1.48	1.41
3	A	202	E1I	C26-N27	3.34	1.45	1.37
3	F	201	E1I	C13-N12	3.34	1.48	1.41
3	E	201	E1I	C26-N27	3.27	1.45	1.37
3	D	201	E1I	C13-N12	3.16	1.47	1.41
3	C	201	E1I	C34-N32	-3.15	1.32	1.35
3	A	202	E1I	C34-N32	-3.06	1.32	1.35
3	B	201	E1I	C03-N02	2.98	1.44	1.39
3	C	201	E1I	C03-N02	2.93	1.44	1.39
3	A	202	E1I	C13-N12	2.82	1.47	1.41
3	F	201	E1I	C34-N32	-2.62	1.33	1.35
3	C	201	E1I	C13-N12	2.59	1.46	1.41
3	A	202	E1I	C03-N02	2.52	1.44	1.39
3	F	201	E1I	C03-N02	2.49	1.43	1.39
3	B	201	E1I	C34-N32	-2.47	1.33	1.35
3	D	201	E1I	C03-N02	2.46	1.43	1.39
3	A	202	E1I	C05-C03	2.43	1.53	1.47
3	B	201	E1I	C07-C06	2.42	1.42	1.38
3	D	201	E1I	C05-C03	2.35	1.52	1.47
3	E	201	E1I	C07-C06	2.32	1.42	1.38
3	F	201	E1I	C05-C03	2.31	1.52	1.47
3	F	201	E1I	O40-C39	2.26	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	E1I	C05-C03	2.24	1.52	1.47
3	B	201	E1I	O11-C10	-2.22	1.18	1.23
3	E	201	E1I	C03-N02	2.19	1.43	1.39
3	D	201	E1I	C21-N20	2.18	1.50	1.46
3	C	201	E1I	C05-C03	2.17	1.52	1.47
3	D	201	E1I	C07-C06	2.16	1.41	1.38
3	D	201	E1I	O40-C39	2.12	1.41	1.37
3	D	201	E1I	C34-N32	-2.06	1.33	1.35

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	201	E1I	C26-N27-C28	-6.56	119.55	125.94
3	E	201	E1I	C18-C17-N16	-6.48	117.28	122.84
3	F	201	E1I	C26-N27-C28	-5.97	120.12	125.94
3	E	201	E1I	C26-N27-C28	-5.76	120.33	125.94
3	C	201	E1I	C18-C17-N16	-5.62	118.02	122.84
3	E	201	E1I	C29-C28-N02	5.55	125.50	119.02
3	A	202	E1I	C18-C17-N16	-5.48	118.14	122.84
3	D	201	E1I	C26-N27-C28	-5.34	120.74	125.94
3	D	201	E1I	C18-C17-N16	-5.32	118.27	122.84
3	E	201	E1I	C33-N32-N31	5.25	126.68	120.50
3	F	201	E1I	C33-N32-N31	5.13	126.53	120.50
3	F	201	E1I	C30-N31-N32	5.13	109.57	104.23
3	B	201	E1I	C18-C17-N16	-5.07	118.49	122.84
3	A	202	E1I	C26-N27-C28	-5.05	121.02	125.94
3	B	201	E1I	C26-N27-C28	-5.04	121.03	125.94
3	F	201	E1I	C18-C17-N16	-4.99	118.55	122.84
3	D	201	E1I	C30-N31-N32	4.97	109.41	104.23
3	B	201	E1I	C30-N31-N32	4.93	109.36	104.23
3	F	201	E1I	C29-C28-N02	4.83	124.66	119.02
3	E	201	E1I	C13-C18-CL19	-4.80	114.07	119.54
3	E	201	E1I	C30-N31-N32	4.67	109.09	104.23
3	A	202	E1I	C33-N32-N31	4.48	125.77	120.50
3	A	202	E1I	C14-C15-N20	-4.29	117.19	122.29
3	D	201	E1I	C14-C15-N20	-4.19	117.31	122.29
3	D	201	E1I	C33-N32-N31	4.02	125.23	120.50
3	A	202	E1I	C30-N31-N32	3.95	108.34	104.23
3	F	201	E1I	C17-C18-C13	3.87	122.31	120.06
3	E	201	E1I	C17-C18-CL19	3.79	123.75	118.60
3	C	201	E1I	C30-N31-N32	3.75	108.14	104.23
3	B	201	E1I	C29-C28-N02	3.66	123.29	119.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	202	E1I	C29-C28-N02	3.64	123.27	119.02
3	E	201	E1I	C17-C18-C13	3.60	122.16	120.06
3	D	201	E1I	C29-C28-N02	3.60	123.22	119.02
3	B	201	E1I	C33-N32-N31	3.57	124.70	120.50
3	D	201	E1I	C17-C18-C13	3.57	122.14	120.06
3	E	201	E1I	C34-N32-N31	-3.56	108.46	111.56
3	C	201	E1I	C35-C42-C41	-3.52	118.37	121.53
3	C	201	E1I	C14-C15-N20	-3.51	118.11	122.29
3	F	201	E1I	C34-N32-N31	-3.50	108.51	111.56
3	A	202	E1I	C25-N20-C21	-3.39	104.03	111.52
3	B	201	E1I	C13-C18-CL19	-3.36	115.71	119.54
3	E	201	E1I	C05-C03-N02	3.33	120.18	115.74
3	B	201	E1I	C17-C18-C13	3.29	121.98	120.06
3	B	201	E1I	C14-C15-N20	-3.18	118.51	122.29
3	B	201	E1I	C05-C03-N02	3.15	119.94	115.74
3	F	201	E1I	C05-C03-N02	3.14	119.92	115.74
3	D	201	E1I	C34-N32-N31	-3.12	108.84	111.56
3	C	201	E1I	C33-N32-N31	3.11	124.16	120.50
3	E	201	E1I	C14-C15-N20	-3.10	118.61	122.29
3	E	201	E1I	C17-N16-C15	3.10	122.95	117.30
3	D	201	E1I	C05-C03-N02	3.09	119.85	115.74
3	C	201	E1I	C13-C18-CL19	-3.01	116.11	119.54
3	A	202	E1I	C05-C03-N02	3.00	119.74	115.74
3	D	201	E1I	C25-N20-C21	-2.97	104.96	111.52
3	C	201	E1I	C17-C18-C13	2.95	121.78	120.06
3	F	201	E1I	C14-C15-N20	-2.87	118.89	122.29
3	C	201	E1I	C17-N16-C15	2.86	122.52	117.30
3	A	202	E1I	N16-C15-N20	2.85	121.05	116.79
3	A	202	E1I	C17-N16-C15	2.85	122.49	117.30
3	B	201	E1I	C36-C37-C39	2.80	120.37	118.08
3	F	201	E1I	C13-C18-CL19	-2.75	116.41	119.54
3	A	202	E1I	C34-N32-N31	-2.73	109.18	111.56
3	F	201	E1I	C35-C42-C41	-2.73	119.07	121.53
3	C	201	E1I	C05-C03-N02	2.73	119.38	115.74
3	B	201	E1I	C17-C18-CL19	2.71	122.28	118.60
3	D	201	E1I	C36-C37-C39	2.70	120.29	118.08
3	C	201	E1I	C29-C28-N02	2.69	122.15	119.02
3	B	201	E1I	C34-N32-N31	-2.67	109.23	111.56
3	D	201	E1I	C21-N20-C15	-2.66	114.20	120.39
3	B	201	E1I	C17-N16-C15	2.66	122.16	117.30
3	C	201	E1I	C17-C18-CL19	2.56	122.08	118.60
3	A	202	E1I	C35-C42-C41	-2.52	119.26	121.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	201	E1I	C25-N20-C21	-2.52	105.96	111.52
3	B	201	E1I	C35-C36-C37	-2.51	119.36	122.33
3	C	201	E1I	C24-O23-C22	2.46	118.10	109.89
3	D	201	E1I	C35-C42-C41	-2.43	119.35	121.53
3	D	201	E1I	C17-N16-C15	2.43	121.73	117.30
3	D	201	E1I	C35-C36-C37	-2.43	119.46	122.33
3	E	201	E1I	C35-C42-C41	-2.41	119.36	121.53
3	D	201	E1I	C13-C18-CL19	-2.41	116.80	119.54
3	D	201	E1I	N16-C15-N20	2.38	120.35	116.79
3	A	202	E1I	C17-C18-C13	2.34	121.42	120.06
3	B	201	E1I	O04-C03-C05	-2.34	119.89	124.25
3	B	201	E1I	C22-C21-N20	2.31	114.28	110.02
3	F	201	E1I	C36-C37-C39	2.28	119.94	118.08
3	A	202	E1I	C21-N20-C15	-2.26	115.13	120.39
3	F	201	E1I	C17-N16-C15	2.25	121.40	117.30
3	F	201	E1I	C35-C36-C37	-2.24	119.68	122.33
3	E	201	E1I	C35-C36-C37	-2.24	119.69	122.33
3	F	201	E1I	C42-C41-C39	2.17	121.32	119.00
3	C	201	E1I	C42-C41-C39	2.15	121.30	119.00
3	E	201	E1I	C25-N20-C21	-2.07	106.95	111.52
3	B	201	E1I	C35-C42-C41	-2.01	119.72	121.53

There are no chirality outliers.

All (8) torsion outliers are listed below:

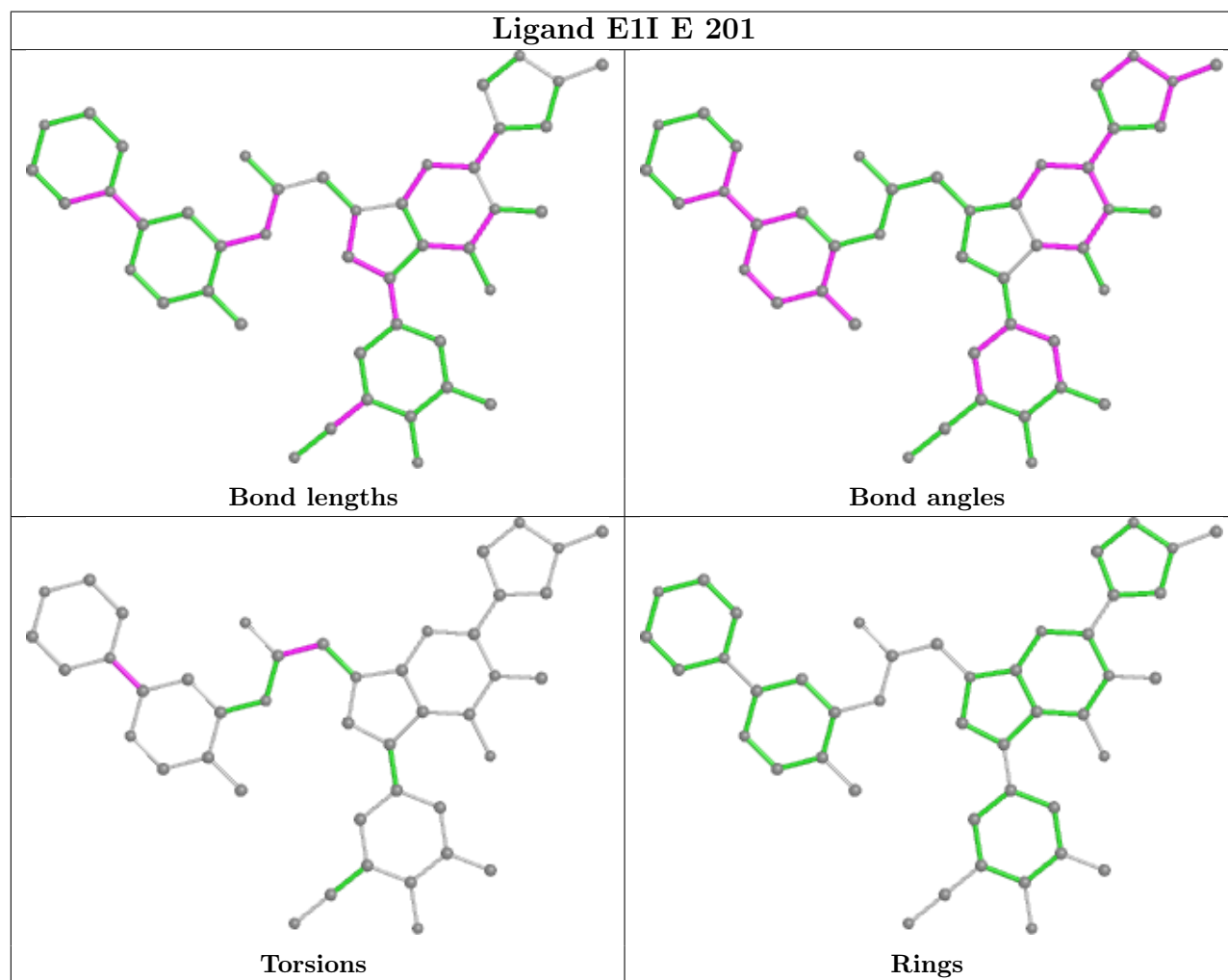
Mol	Chain	Res	Type	Atoms
3	E	201	E1I	N08-C09-C10-N12
3	E	201	E1I	N08-C09-C10-O11
3	D	201	E1I	N16-C15-N20-C21
3	E	201	E1I	N16-C15-N20-C21
3	F	201	E1I	N08-C09-C10-N12
3	A	202	E1I	N16-C15-N20-C21
3	E	201	E1I	C14-C15-N20-C21
3	D	201	E1I	C14-C15-N20-C21

There are no ring outliers.

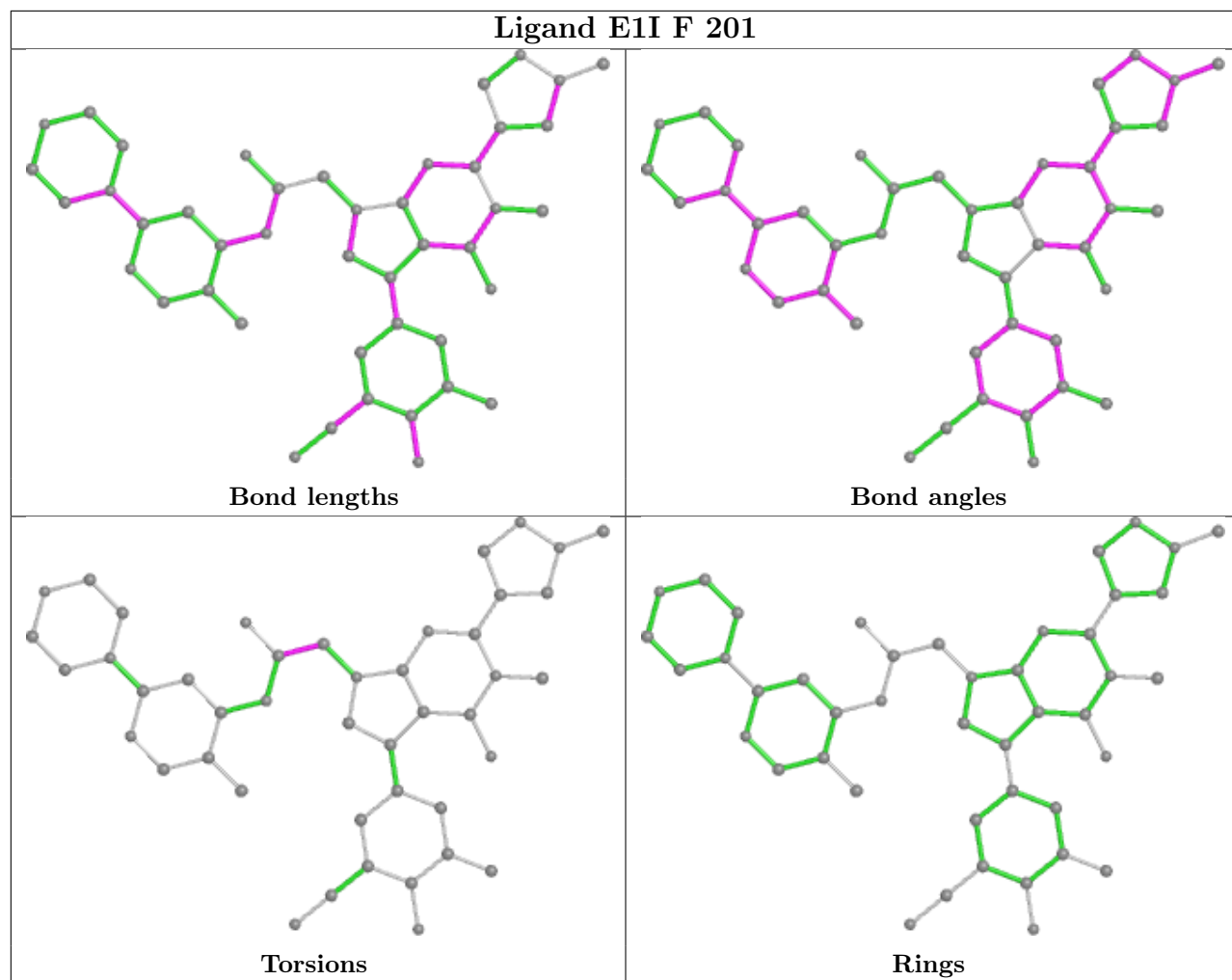
2 monomers are involved in 3 short contacts:

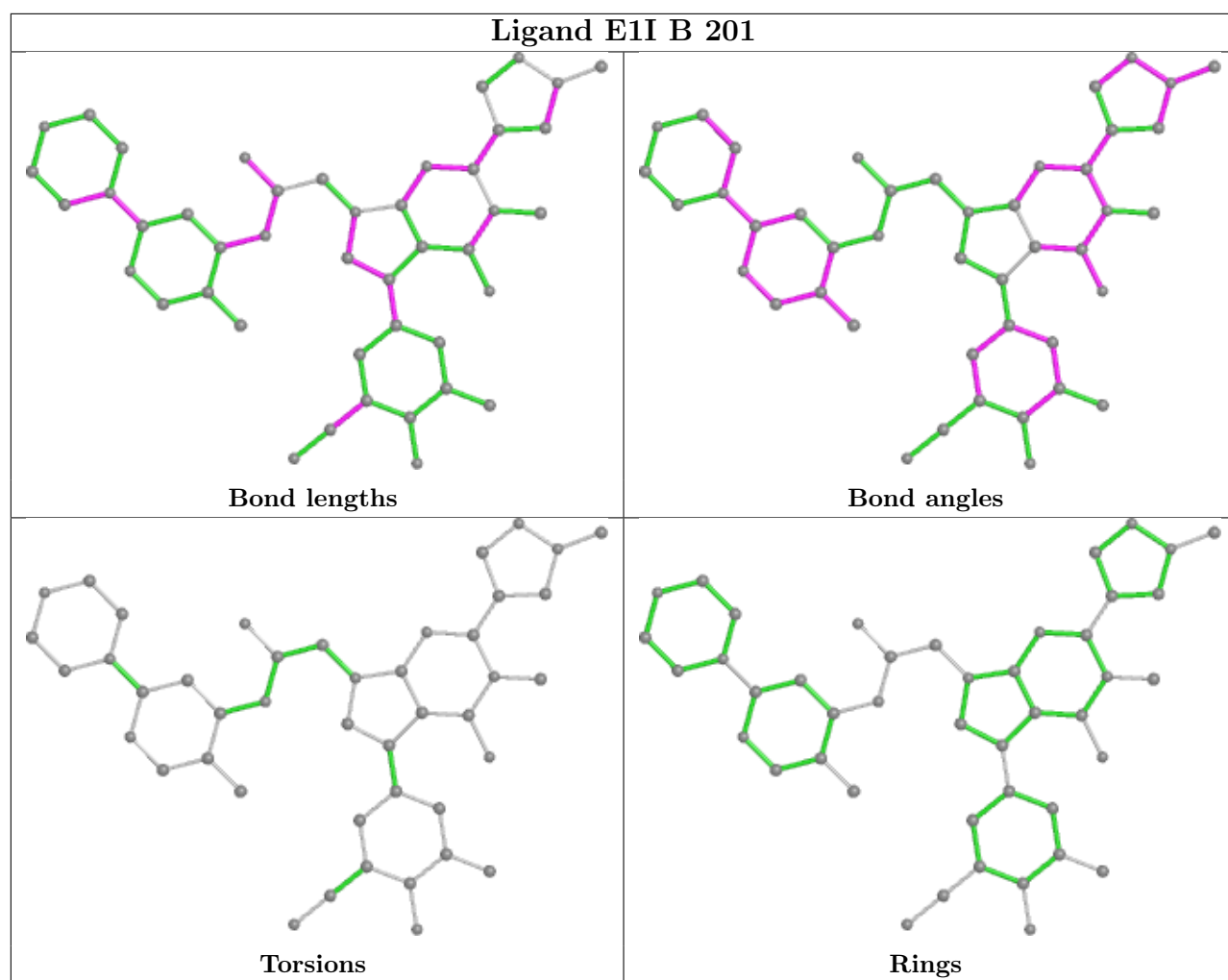
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	201	E1I	1	0
3	F	201	E1I	2	0

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.

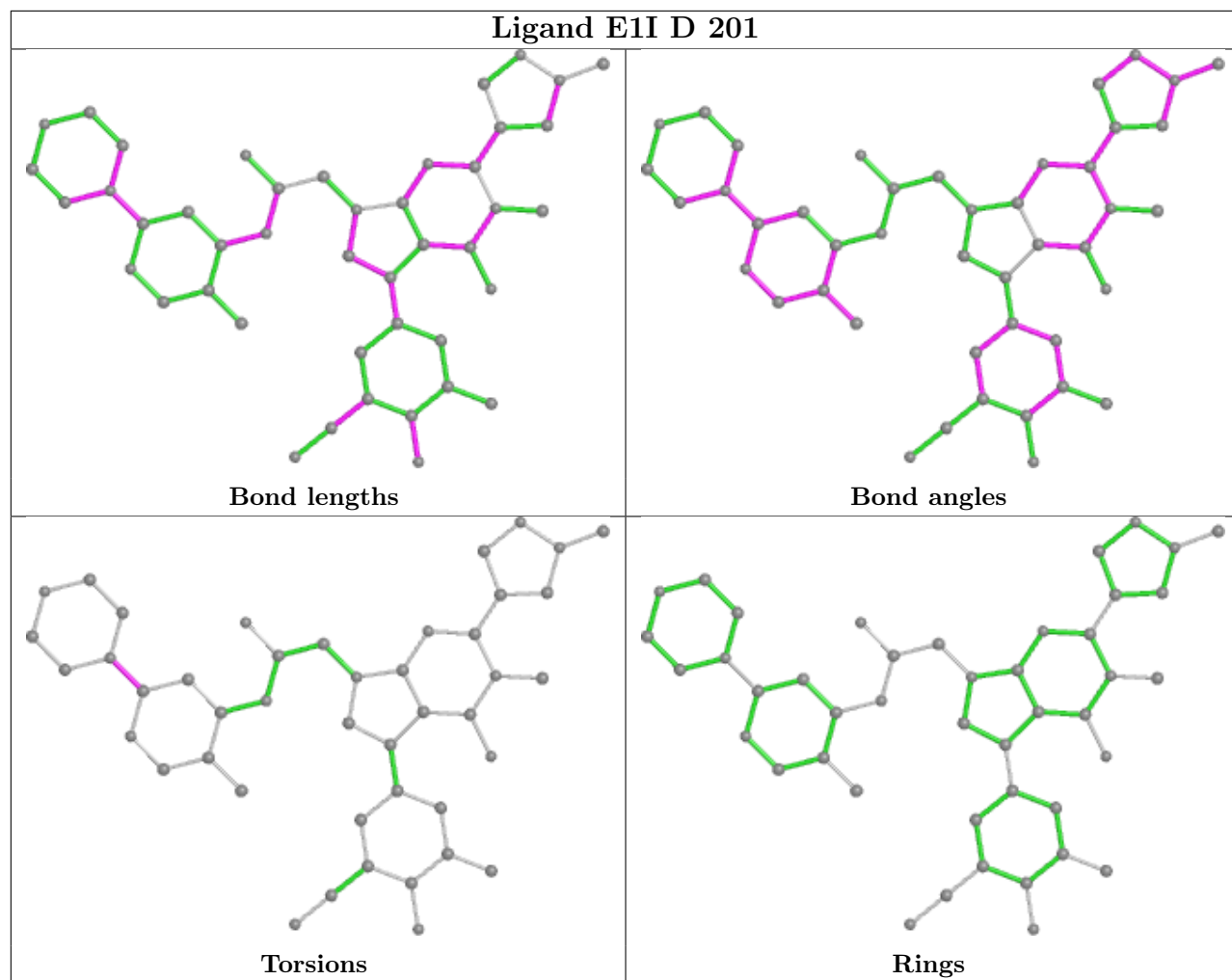


Ligand E1I F 201

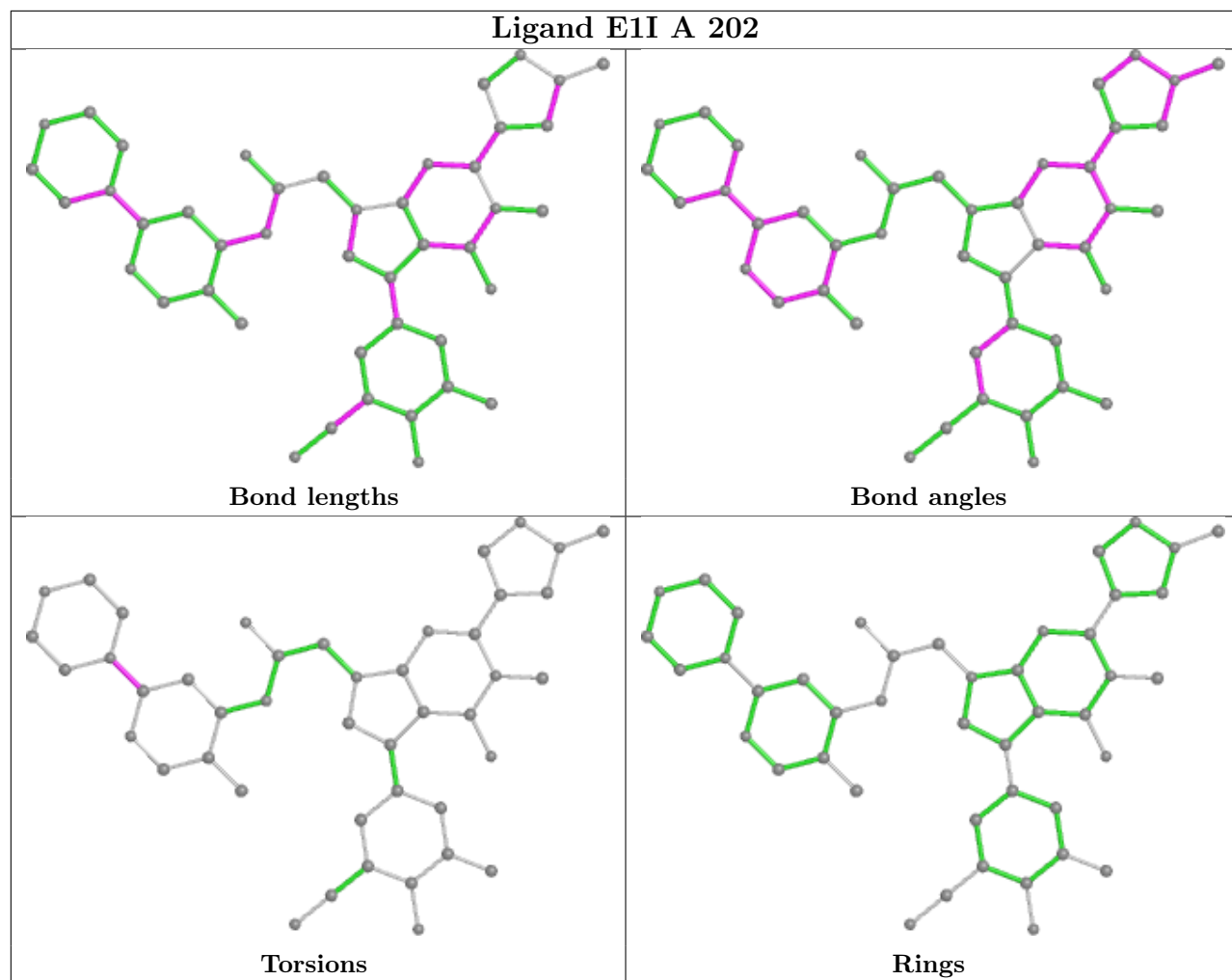


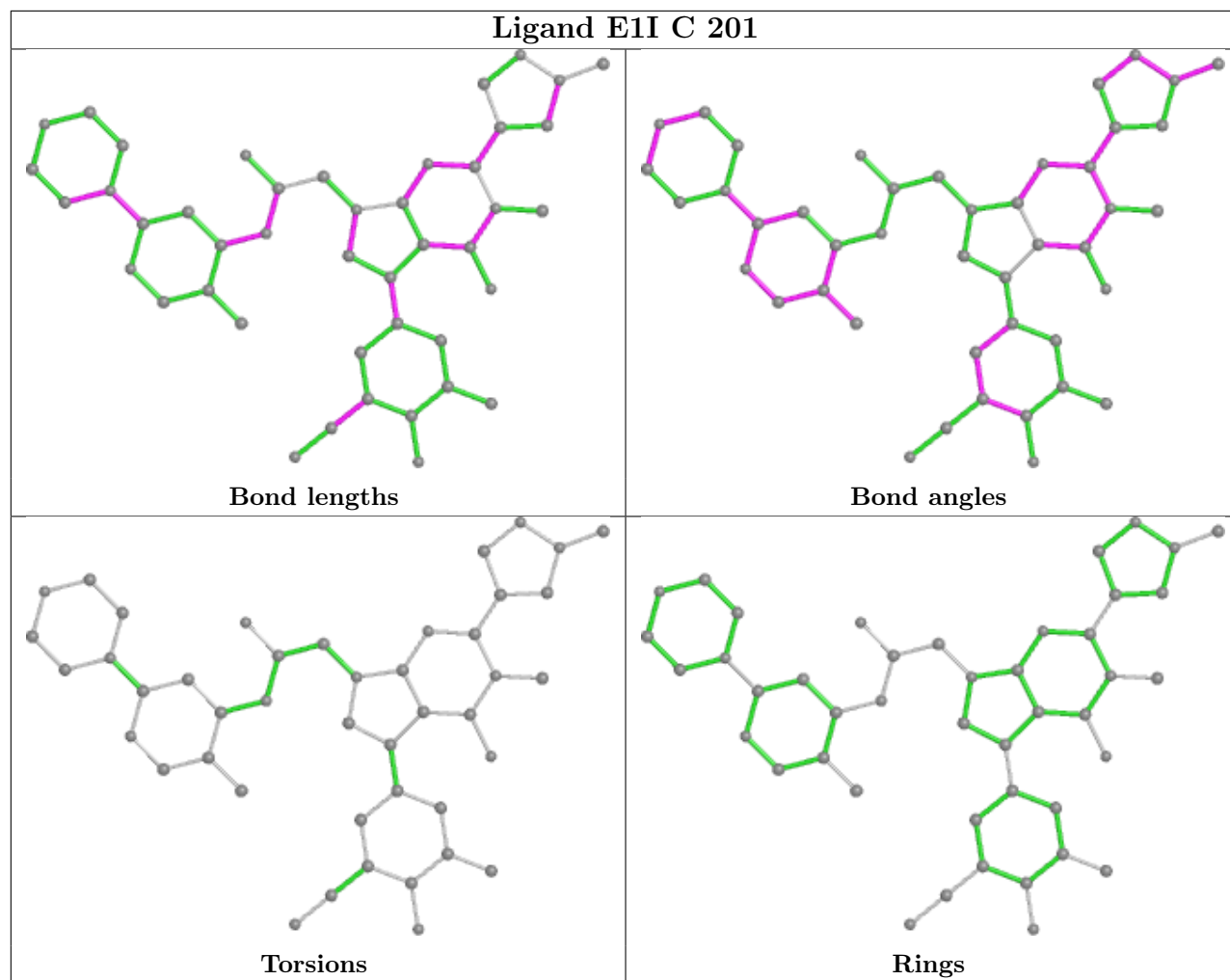


Ligand E1I D 201



Ligand E1I A 202





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	123/127 (96%)	-0.06	2 (1%) 72 70	13, 22, 56, 67	0
1	B	122/127 (96%)	0.05	4 (3%) 46 45	13, 24, 54, 75	0
1	C	123/127 (96%)	0.01	6 (4%) 29 28	13, 24, 48, 84	0
1	D	121/127 (95%)	0.14	10 (8%) 11 10	14, 24, 61, 78	0
1	E	122/127 (96%)	0.25	8 (6%) 18 17	14, 26, 58, 68	0
1	F	122/127 (96%)	0.12	5 (4%) 37 36	14, 29, 61, 77	0
All	All	733/762 (96%)	0.08	35 (4%) 30 29	13, 25, 59, 84	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	65	LEU	5.6
1	C	7	SER	5.0
1	D	40	ARG	4.8
1	A	128	SER	4.3
1	E	127	ALA	4.2
1	B	128	SER	4.0
1	D	98	ARG	3.8
1	C	124	PHE	3.1
1	D	124	PHE	3.1
1	E	9	ILE	3.1
1	F	7	SER	3.1
1	D	99	GLU	3.1
1	E	124	PHE	3.1
1	D	128	SER	3.0
1	D	68	ASN	3.0
1	A	127	ALA	3.0
1	D	76	PRO	2.8
1	D	96	ASN	2.8
1	F	76	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	126	LYS	2.7
1	E	97	LEU	2.7
1	F	103	MET	2.6
1	D	5	ALA	2.6
1	B	65	LEU	2.6
1	D	67	ARG	2.5
1	C	128	SER	2.5
1	C	44[A]	ARG	2.5
1	B	96	ASN	2.5
1	F	70	SER	2.4
1	C	123	LYS	2.4
1	F	97	LEU	2.3
1	E	100	GLY	2.3
1	C	40	ARG	2.3
1	B	66	LYS	2.2
1	E	66	LYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DMS	A	201	4/4	0.83	0.20	21,26,31,34	10
2	DMS	E	202	4/4	0.94	0.19	23,27,32,39	10
3	E1I	C	201	44/44	0.94	0.15	14,17,22,27	0
3	E1I	B	201	44/44	0.95	0.13	14,17,22,25	0
3	E1I	D	201	44/44	0.95	0.14	14,17,24,27	0
3	E1I	A	202	44/44	0.96	0.14	14,16,26,30	0
3	E1I	F	201	44/44	0.96	0.14	12,18,22,25	0

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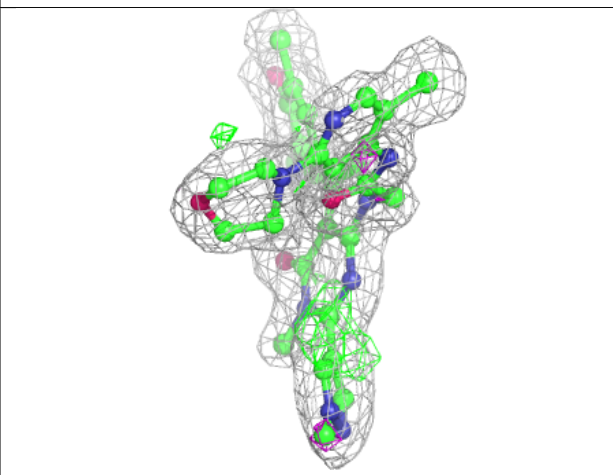
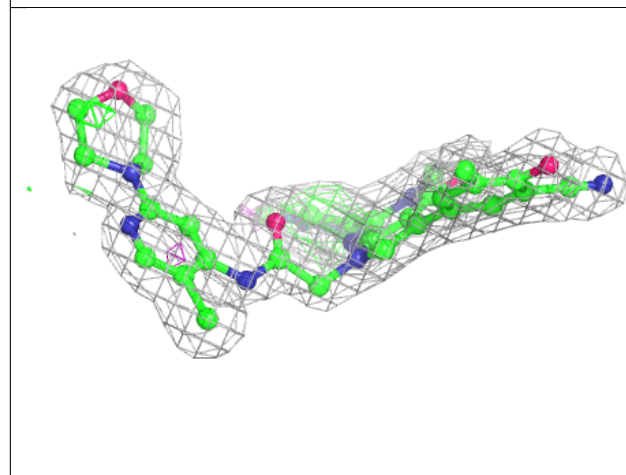
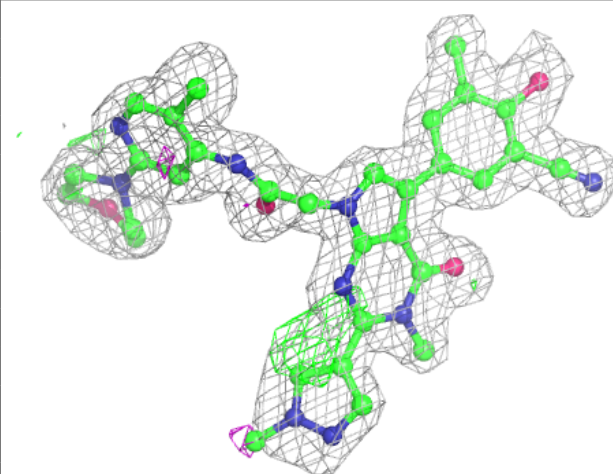
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	E1I	E	201	44/44	0.97	0.14	11,15,20,22	0

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.

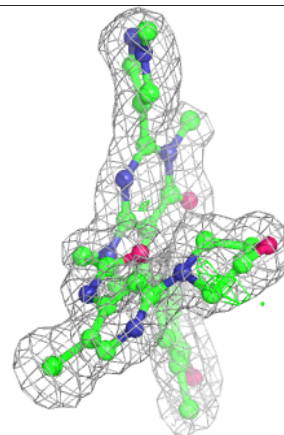
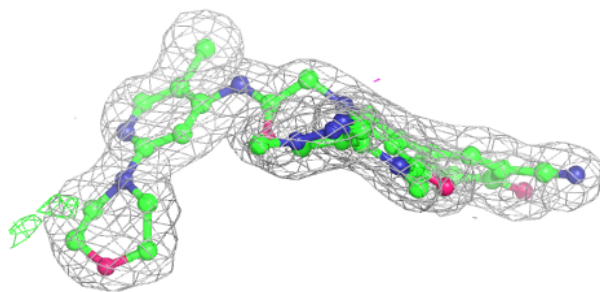
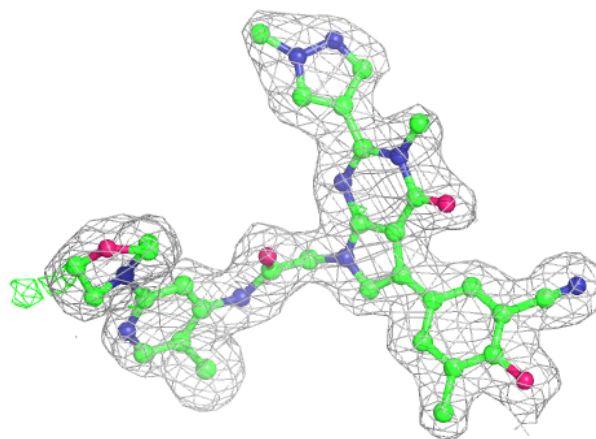
Electron density around E1I C 201:

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



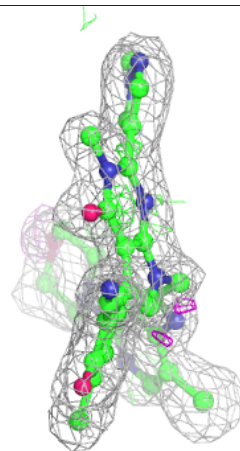
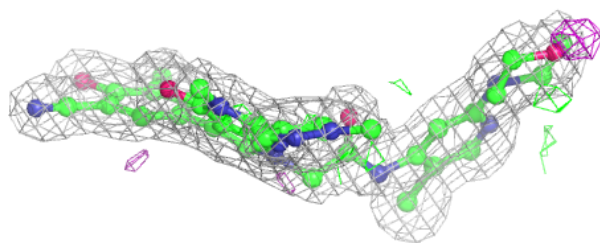
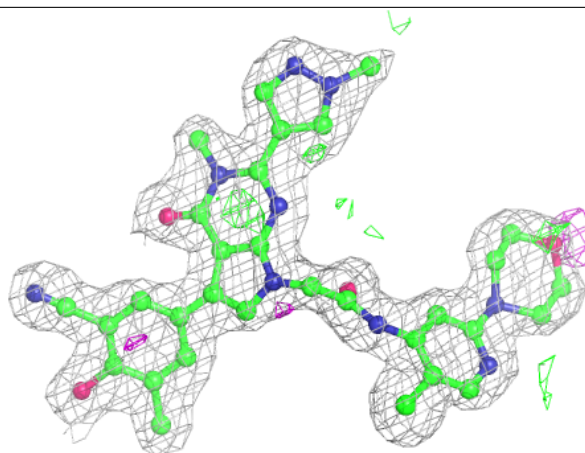
Electron density around E1I B 201:

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



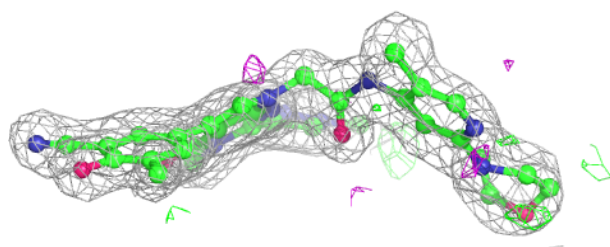
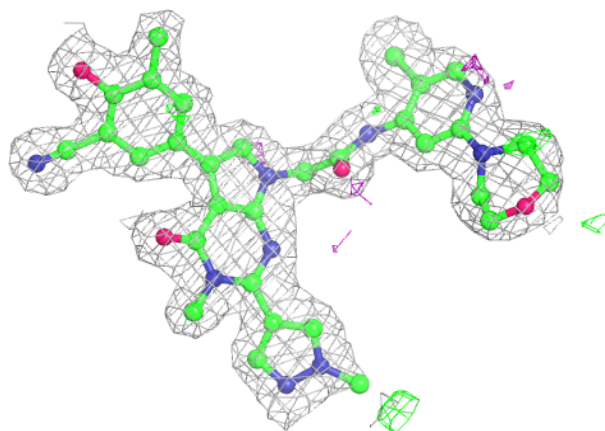
Electron density around E1I D 201:

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



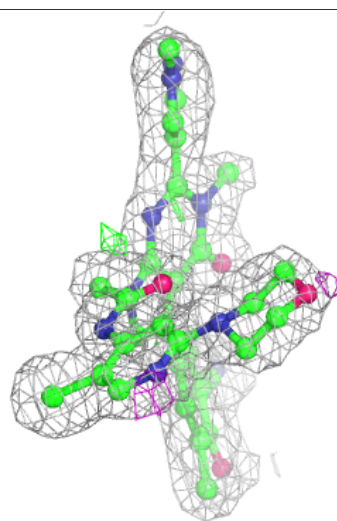
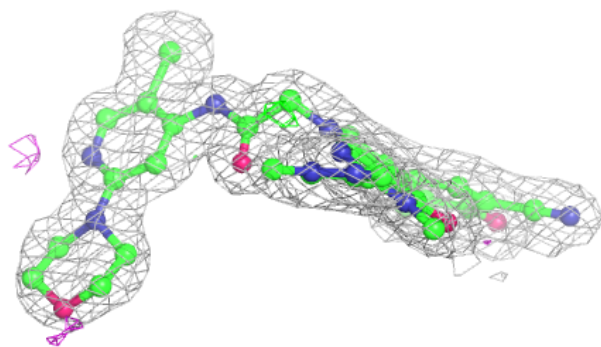
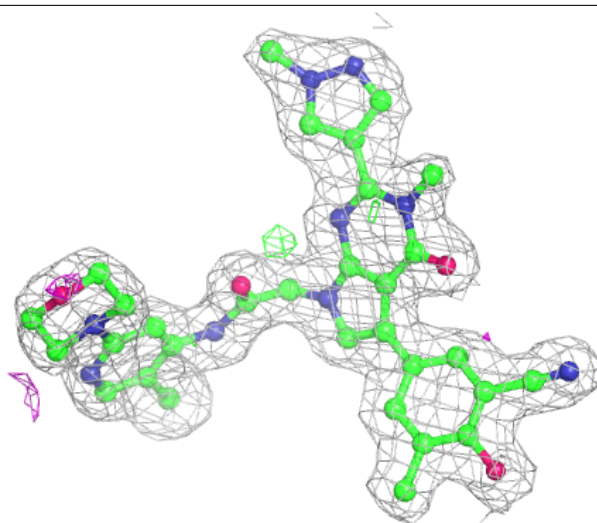
Electron density around E1I A 202:

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



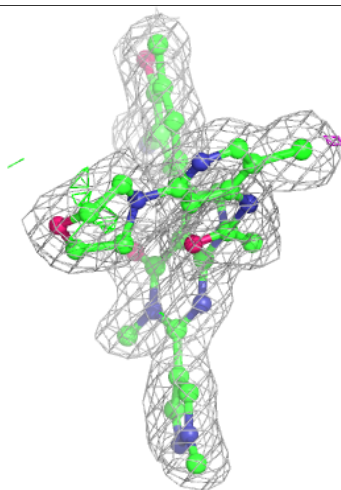
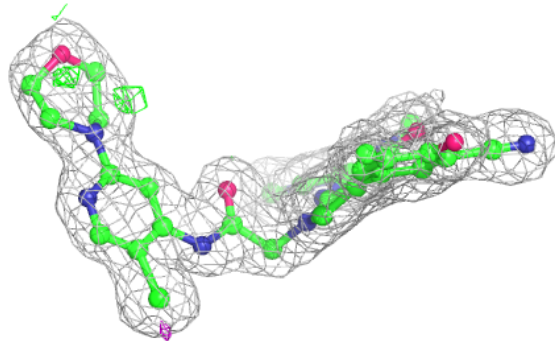
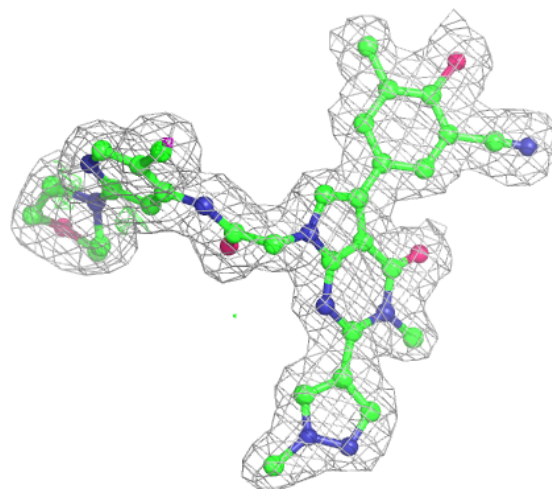
Electron density around E1I F 201:

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



Electron density around E11 E 201:

$2mF_o-DF_c$ (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.