W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 20, 2020 – 02:18 am BST

PDB ID	:	3E8E
Title	:	Crystal structures of the kinase domain of PKA in complex with ATP-competitive inhibitors
Authors	:	Concha, N.O.; Elkins, P.A.; Smallwood, A.; Ward, P.
Deposited on	:	2008-08-19
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references ⓘ) were used in the production of this report:

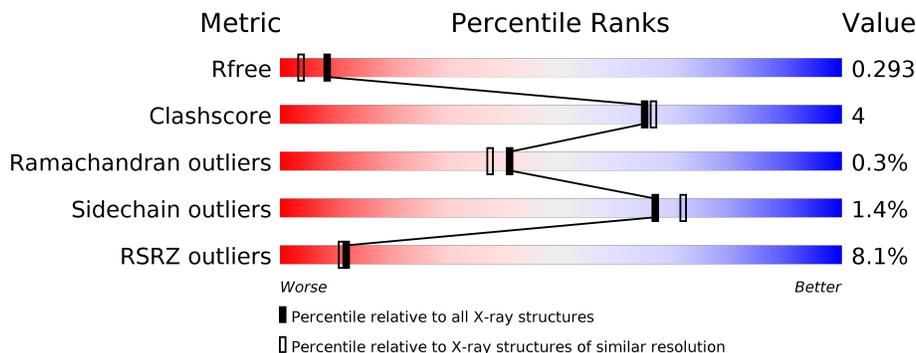|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	Percentile Ranks	Value
Rfree		0.293
Clashscore		4
Ramachandran outliers		0.3%
Sidechain outliers		1.4%
RSRZ outliers		8.1%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

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 on 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 <=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	350	5% / 89% / 9% ·
1	B	350	7% / 90% / 7% ·
1	E	350	5% / 85% / 13% ··
1	I	350	3% / 92% / 7% ·
1	L	350	11% / 87% / 9% ·
1	P	350	11% / 90% / 8% ·

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Mol	Chain	Length	Quality of chain
2	C	20	35% / 70% / 30%
2	F	20	15% / 70% / 30%
2	G	20	20% / 80% / 15% / 5%
2	J	20	25% / 90% / 10%
2	N	20	10% / 90% / 10%
2	Q	20	30% / 80% / 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18474 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 cAMP-dependent protein kinase catalytic subunit alpha.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	344	Total 2848	C 1840	N 477	O 519	P 3	S 9	0	1	0
1	B	339	Total 2804	C 1816	N 469	O 508	P 2	S 9	0	1	0
1	E	344	Total 2840	C 1834	N 475	O 519	P 3	S 9	0	1	0
1	I	348	Total 2858	C 1845	N 478	O 523	P 3	S 9	0	1	0
1	L	338	Total 2798	C 1813	N 468	O 506	P 2	S 9	0	1	0
1	P	344	Total 2844	C 1837	N 475	O 520	P 3	S 9	0	2	0

- Molecule 2 is a protein called PKI inhibitor peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	20	Total 157	C 94	N 32	O 31	0	0	0
2	C	20	Total 157	C 94	N 32	O 31	0	0	0
2	F	20	Total 157	C 94	N 32	O 31	0	0	0
2	J	20	Total 157	C 94	N 32	O 31	0	0	0
2	N	20	Total 157	C 94	N 32	O 31	0	0	0
2	Q	20	Total 157	C 94	N 32	O 31	0	0	0

- Molecule 3 is 4-[2-(4-amino-2,5-dihydro-1,2,5-oxadiazol-3-yl)-6-{[(1S)-3-amino-1-phenylpropyl]oxy}-1-ethyl-1H-imidazo[4,5-c]pyridin-4-yl]-2-methylbut-3-yn-2-ol (three-letter code: G98) (formula: $C_{24}H_{29}N_7O_3$).

G98
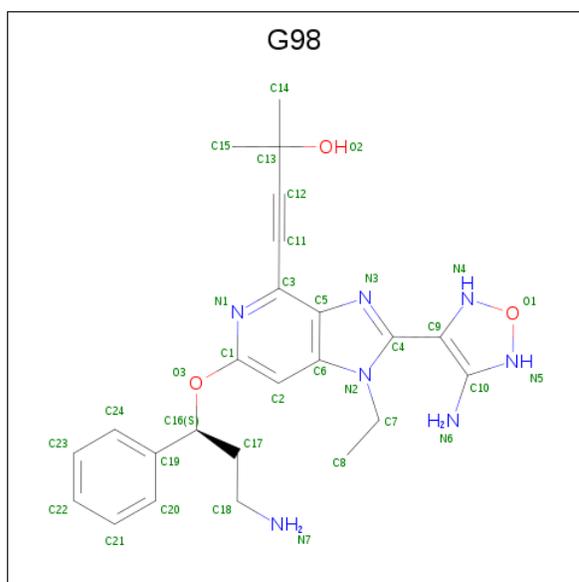
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			34	24	7	3		
3	B	1	Total	C	N	O	0	0
			34	24	7	3		
3	E	1	Total	C	N	O	0	0
			34	24	7	3		
3	I	1	Total	C	N	O	0	0
			34	24	7	3		
3	L	1	Total	C	N	O	0	0
			34	24	7	3		
3	P	1	Total	C	N	O	0	0
			34	24	7	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	74	Total	O	0	0
			74	74		
4	G	3	Total	O	0	0
			3	3		
4	B	65	Total	O	0	0
			65	65		
4	C	4	Total	O	0	0
			4	4		
4	E	76	Total	O	0	0
			76	76		
4	F	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	I	38	Total 38	O 38	0	0
4	J	2	Total 2	O 2	0	0
4	L	41	Total 41	O 41	0	0
4	N	4	Total 4	O 4	0	0
4	P	26	Total 26	O 26	0	0
4	Q	1	Total 1	O 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.
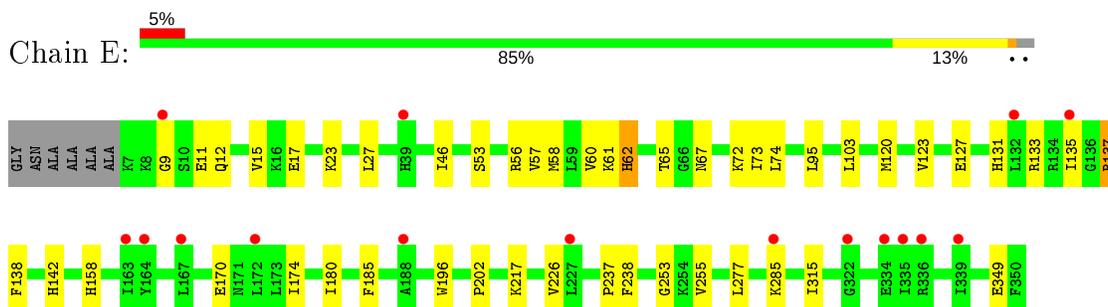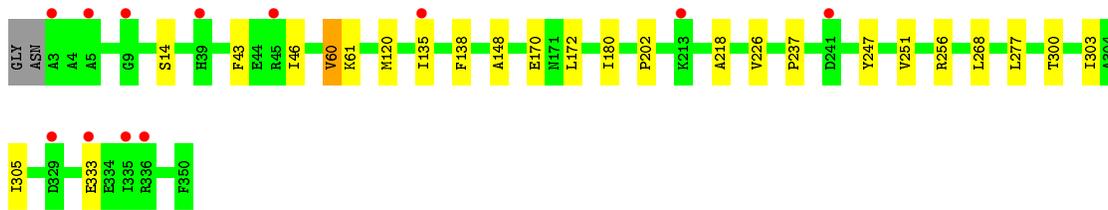
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha
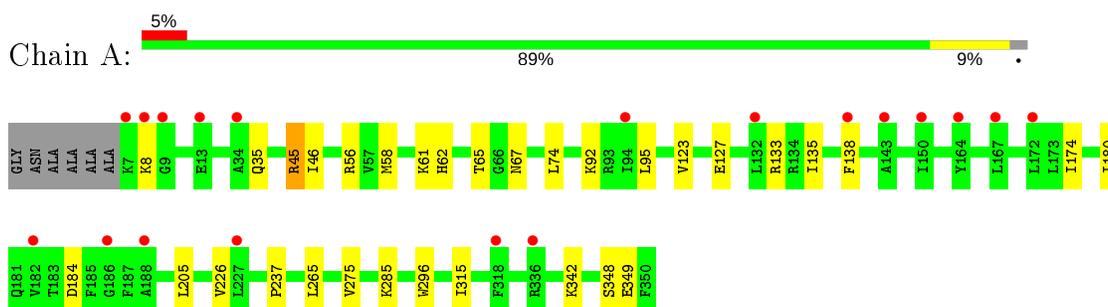
- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

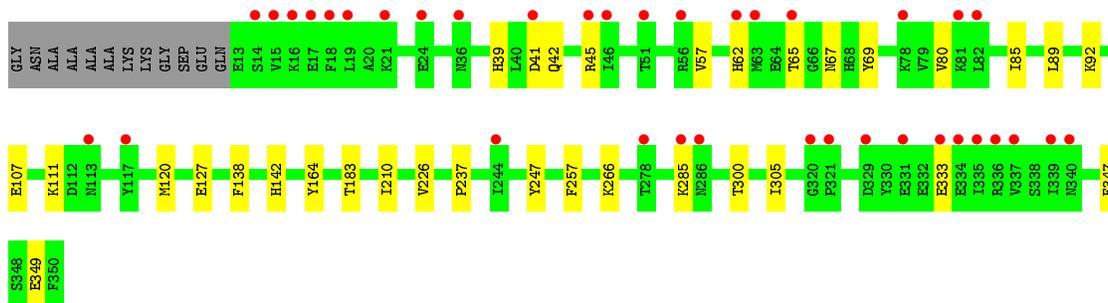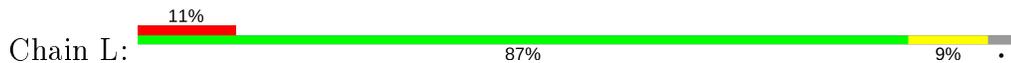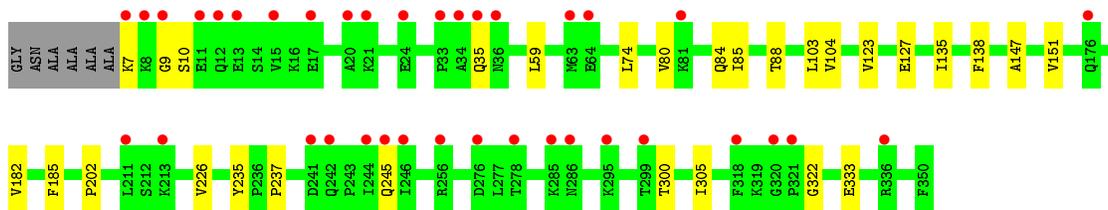- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

- Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha
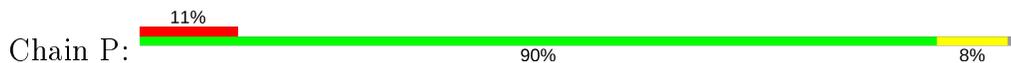
• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha

Chain L:

• Molecule 1: cAMP-dependent protein kinase catalytic subunit alpha
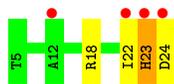
Chain P:

• Molecule 2: PKI inhibitor peptide

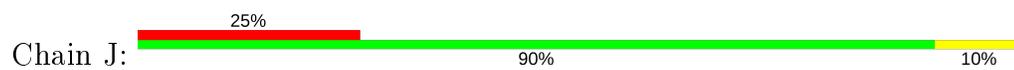Chain G:

• Molecule 2: PKI inhibitor peptide

Chain C:
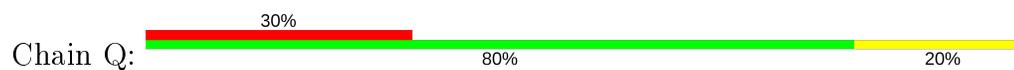

• Molecule 2: PKI inhibitor peptide

Chain F:

• Molecule 2: PKI inhibitor peptide

Chain J:

• Molecule 2: PKI inhibitor peptide

Chain N:

• Molecule 2: PKI inhibitor peptide

Chain Q:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.58Å 95.85Å 179.10Å 90.00° 102.53° 90.00°	Depositor
Resolution (Å)	42.03 – 2.00 42.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.5 (42.03-2.00) 93.5 (42.02-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.279 0.258 , 0.293	Depositor DCC
R_{free} test set	8636 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.5	Xtriage
Anisotropy	0.681	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
L-test for twinning [2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	0.001 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18474	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2535e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: TPO, SEP, G98

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	0.40	0/2890	0.58	1/3888 (0.0%)
1	B	0.39	0/2857	0.58	1/3849 (0.0%)
1	E	0.41	0/2882	0.60	3/3880 (0.1%)
1	I	0.36	0/2900	0.53	0/3906
1	L	0.37	0/2851	0.53	0/3840
1	P	0.37	0/2889	0.52	0/3890
2	C	0.38	0/159	0.69	0/212
2	F	0.43	0/159	0.68	0/212
2	G	0.36	0/159	0.61	0/212
2	J	0.34	0/159	0.60	0/212
2	N	0.36	0/159	0.61	0/212
2	Q	0.42	0/159	0.69	0/212
All	All	0.38	0/18223	0.56	5/24525 (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	E	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	133	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	E	137	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	144	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	133	ARG	NE-CZ-NH2	-5.16	117.72	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	ARG	NE-CZ-NH1	5.09	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	62	HIS	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2848	0	2823	21	0
1	B	2804	0	2776	22	0
1	E	2840	0	2802	36	0
1	I	2858	0	2815	18	0
1	L	2798	0	2777	18	0
1	P	2844	0	2802	18	0
2	C	157	0	146	4	0
2	F	157	0	146	6	0
2	G	157	0	146	3	0
2	J	157	0	146	2	0
2	N	157	0	146	1	0
2	Q	157	0	146	3	0
3	A	34	0	29	6	0
3	B	34	0	29	5	0
3	E	34	0	29	7	0
3	I	34	0	29	2	0
3	L	34	0	29	1	0
3	P	34	0	29	3	0
4	A	74	0	0	1	0
4	B	65	0	0	0	0
4	C	4	0	0	0	0
4	E	76	0	0	1	0
4	F	2	0	0	0	0
4	G	3	0	0	0	0
4	I	38	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	J	2	0	0	0	0
4	L	41	0	0	0	0
4	N	4	0	0	0	0
4	P	26	0	0	0	0
4	Q	1	0	0	0	0
All	All	18474	0	17845	149	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.

The worst 5 of 149 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:B:135:ILE:HD11	1:B:138:PHE:CD1	2.00	0.97
1:A:135:ILE:HD11	1:A:138:PHE:CD1	2.03	0.93
1:E:135:ILE:HD11	1:E:138:PHE:CD1	2.05	0.92
1:B:135:ILE:HD11	1:B:138:PHE:HD1	1.43	0.84
1:E:135:ILE:HD11	1:E:138:PHE:HD1	1.41	0.83

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	340/350 (97%)	332 (98%)	8 (2%)	0	100	100
1	B	336/350 (96%)	327 (97%)	9 (3%)	0	100	100
1	E	340/350 (97%)	327 (96%)	13 (4%)	0	100	100
1	I	344/350 (98%)	333 (97%)	11 (3%)	0	100	100
1	L	335/350 (96%)	327 (98%)	8 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	341/350 (97%)	333 (98%)	7 (2%)	1 (0%)	41	37
2	C	18/20 (90%)	17 (94%)	0	1 (6%)	2	0
2	F	18/20 (90%)	17 (94%)	0	1 (6%)	2	0
2	G	18/20 (90%)	17 (94%)	0	1 (6%)	2	0
2	J	18/20 (90%)	16 (89%)	2 (11%)	0	100	100
2	N	18/20 (90%)	16 (89%)	1 (6%)	1 (6%)	2	0
2	Q	18/20 (90%)	17 (94%)	0	1 (6%)	2	0
All	All	2144/2220 (97%)	2079 (97%)	59 (3%)	6 (0%)	41	37

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	23	HIS
2	Q	23	HIS
2	F	23	HIS
2	G	23	HIS
2	C	23	HIS

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	302/302 (100%)	297 (98%)	5 (2%)	60	65
1	B	298/302 (99%)	297 (100%)	1 (0%)	92	95
1	E	300/302 (99%)	293 (98%)	7 (2%)	50	53
1	I	299/302 (99%)	293 (98%)	6 (2%)	55	58
1	L	298/302 (99%)	292 (98%)	6 (2%)	55	58
1	P	300/302 (99%)	298 (99%)	2 (1%)	84	88
2	C	15/15 (100%)	15 (100%)	0	100	100
2	F	15/15 (100%)	15 (100%)	0	100	100
2	G	15/15 (100%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	J	15/15 (100%)	15 (100%)	0	100	100
2	N	15/15 (100%)	15 (100%)	0	100	100
2	Q	15/15 (100%)	15 (100%)	0	100	100
All	All	1887/1902 (99%)	1860 (99%)	27 (1%)	67	72

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	349	GLU
1	I	120	MET
1	L	333	GLU
1	I	14	SER
1	A	342	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	289	ASN
1	L	39	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	#$|Z| > 2$
1	SEP	P	338	1	8,9,10	1.49	1 (12%)	8,12,14	1.64	2 (25%)
1	TPO	A	197	1	8,10,11	0.74	0	10,14,16	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	TPO	P	197	1	8,10,11	0.76	0	10,14,16	1.08	1 (10%)
1	SEP	A	10	1	8,9,10	1.66	1 (12%)	8,12,14	2.08	2 (25%)
1	SEP	P	10	1	8,9,10	1.69	1 (12%)	8,12,14	1.76	2 (25%)
1	TPO	E	197	1	8,10,11	0.83	0	10,14,16	1.13	1 (10%)
1	SEP	I	338	1	8,9,10	1.55	1 (12%)	8,12,14	1.61	1 (12%)
1	TPO	I	197	1	8,10,11	0.75	0	10,14,16	1.13	1 (10%)
1	SEP	I	10	1	8,9,10	1.62	1 (12%)	8,12,14	3.64	3 (37%)
1	SEP	B	338	1	8,9,10	1.48	1 (12%)	8,12,14	1.60	2 (25%)
1	TPO	B	197	1	8,10,11	0.76	0	10,14,16	0.88	0
1	SEP	E	338	1	8,9,10	1.54	1 (12%)	8,12,14	1.80	1 (12%)
1	TPO	L	197	1	8,10,11	0.76	0	10,14,16	1.12	1 (10%)
1	SEP	E	10	1	8,9,10	1.64	1 (12%)	8,12,14	2.30	1 (12%)
1	SEP	L	338	1	8,9,10	1.62	1 (12%)	8,12,14	1.80	1 (12%)
1	SEP	A	338	1	8,9,10	1.43	1 (12%)	8,12,14	1.50	2 (25%)

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
1	SEP	P	338	1	-	3/5/8/10	-
1	TPO	A	197	1	-	2/9/11/13	-
1	TPO	P	197	1	-	0/9/11/13	-
1	SEP	A	10	1	-	3/5/8/10	-
1	SEP	P	10	1	-	0/5/8/10	-
1	TPO	E	197	1	-	1/9/11/13	-
1	SEP	I	338	1	-	2/5/8/10	-
1	TPO	I	197	1	-	1/9/11/13	-
1	SEP	I	10	1	-	1/5/8/10	-
1	SEP	B	338	1	-	4/5/8/10	-
1	TPO	B	197	1	-	1/9/11/13	-
1	SEP	E	338	1	-	2/5/8/10	-
1	TPO	L	197	1	-	1/9/11/13	-
1	SEP	E	10	1	-	4/5/8/10	-
1	SEP	L	338	1	-	2/5/8/10	-
1	SEP	A	338	1	-	3/5/8/10	-

wwPDB X-ray Structure Validation Summary Report

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	10	SEP	P-O1P	3.65	1.62	1.50
1	A	10	SEP	P-O1P	3.55	1.62	1.50
1	L	338	SEP	P-O1P	3.47	1.61	1.50
1	I	338	SEP	P-O1P	3.42	1.61	1.50
1	E	338	SEP	P-O1P	3.34	1.61	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	10	SEP	OG-CB-CA	9.35	117.24	108.14
1	E	10	SEP	OG-CB-CA	5.79	113.78	108.14
1	A	10	SEP	OG-CB-CA	4.74	112.76	108.14
1	E	338	SEP	OG-CB-CA	4.47	112.50	108.14
1	L	338	SEP	OG-CB-CA	4.38	112.41	108.14

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	P	338	SEP	CA-CB-OG-P
1	A	197	TPO	O-C-CA-CB
1	A	197	TPO	CB-OG1-P-O3P
1	A	10	SEP	CB-OG-P-O1P
1	A	10	SEP	CB-OG-P-O2P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	P	10	SEP	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	G98	E	351	-	29,37,37	2.11	1 (3%)	36,53,53	1.74	6 (16%)
3	G98	L	351	-	29,37,37	2.20	1 (3%)	36,53,53	1.48	7 (19%)
3	G98	B	351	-	29,37,37	2.18	1 (3%)	36,53,53	1.72	9 (25%)
3	G98	I	351	-	29,37,37	2.16	1 (3%)	36,53,53	1.61	7 (19%)
3	G98	P	351	-	29,37,37	2.17	1 (3%)	36,53,53	1.42	6 (16%)
3	G98	A	351	-	29,37,37	2.28	1 (3%)	36,53,53	1.66	6 (16%)

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	G98	E	351	-	-	6/16/33/33	0/4/4/4
3	G98	L	351	-	-	6/16/33/33	0/4/4/4
3	G98	B	351	-	-	12/16/33/33	0/4/4/4
3	G98	I	351	-	-	7/16/33/33	0/4/4/4
3	G98	P	351	-	-	7/16/33/33	0/4/4/4
3	G98	A	351	-	-	7/16/33/33	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	351	G98	C3-C11	-11.55	1.28	1.43
3	L	351	G98	C3-C11	-11.07	1.28	1.43
3	B	351	G98	C3-C11	-11.02	1.28	1.43
3	P	351	G98	C3-C11	-10.98	1.29	1.43
3	I	351	G98	C3-C11	-10.83	1.29	1.43

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	351	G98	O3-C1-C2	4.89	122.31	116.09
3	E	351	G98	O3-C16-C17	4.72	112.72	105.18
3	I	351	G98	C7-N2-C4	4.23	131.78	126.69
3	E	351	G98	C2-C1-N1	-4.22	119.16	124.09
3	A	351	G98	O3-C1-C2	4.13	121.34	116.09

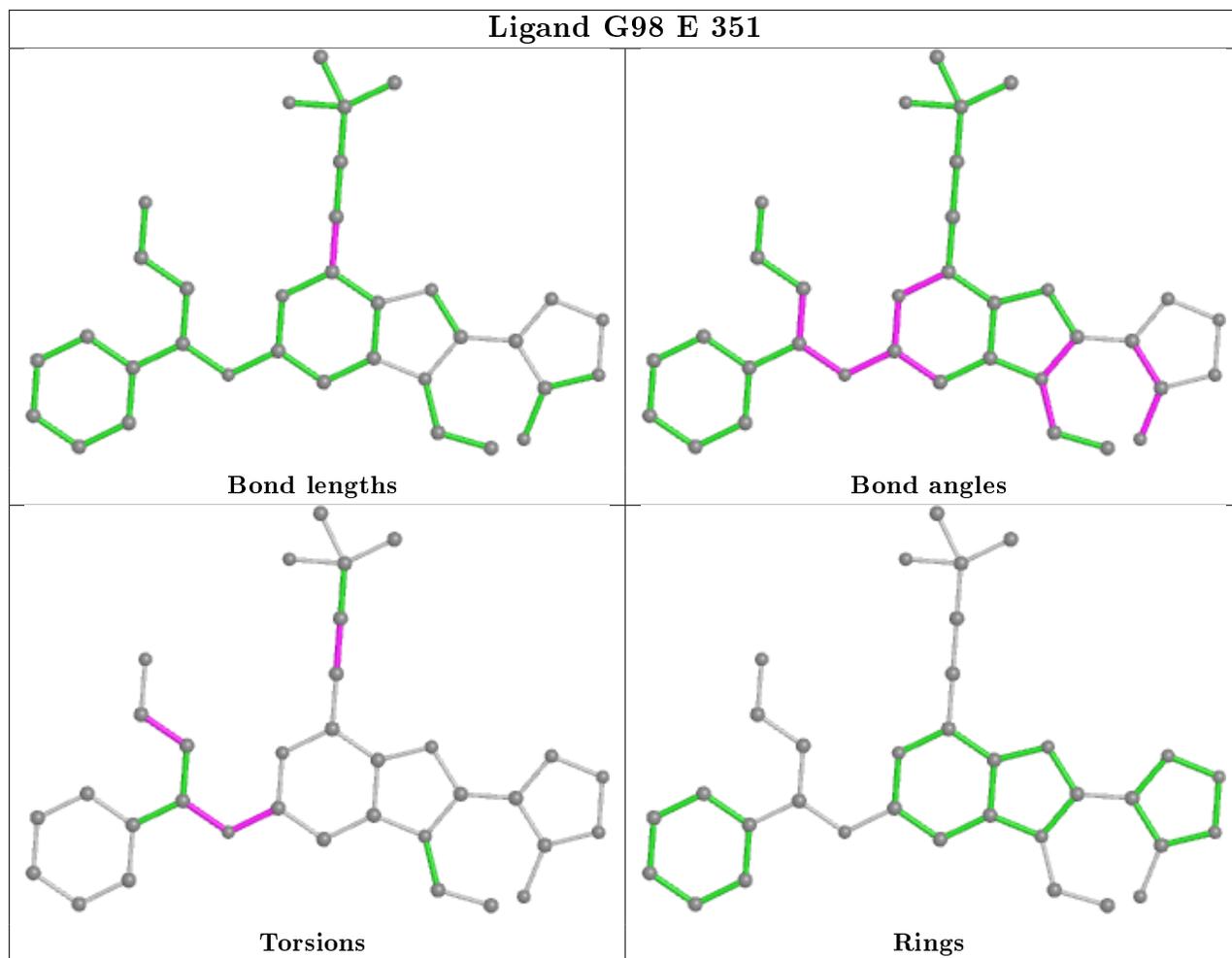There are no chirality outliers.

5 of 45 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	351	G98	C16-C17-C18-N7
3	E	351	G98	N1-C1-O3-C16
3	E	351	G98	C2-C1-O3-C16
3	E	351	G98	C17-C16-O3-C1
3	E	351	G98	C19-C16-O3-C1

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	351	G98	7	0
3	L	351	G98	1	0
3	B	351	G98	5	0
3	I	351	G98	2	0
3	P	351	G98	3	0
3	A	351	G98	6	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 then 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.
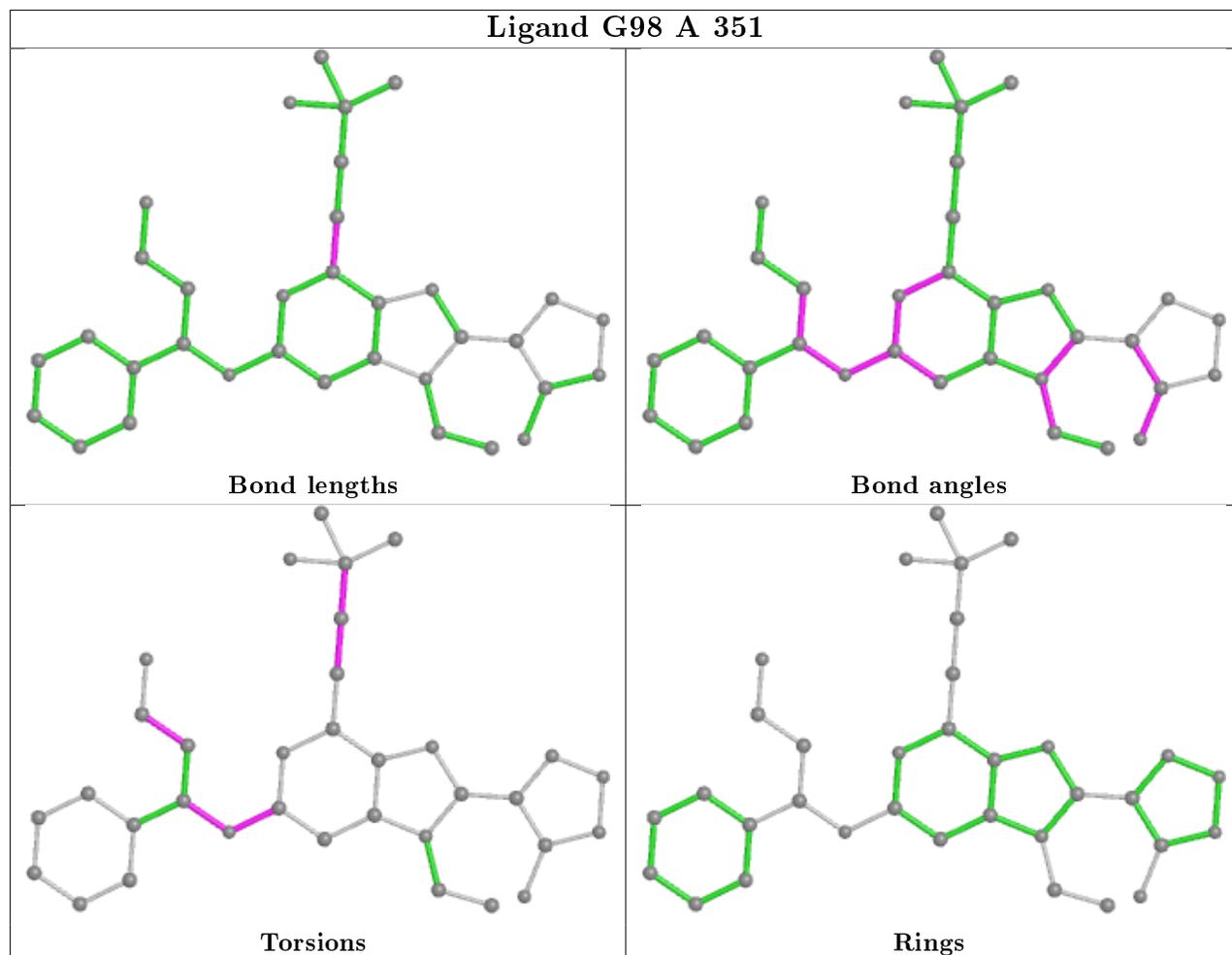
Ligand G98 E 351

Bond lengths

Bond angles

Torsions

Rings

Ligand G98 L 351

Bond lengths

Bond angles

Torsions

Rings

Ligand G98 B 351

Bond lengths

Bond angles

Torsions

Rings

Ligand G98 I 351

Bond lengths

Bond angles

Torsions

Rings

Ligand G98 P 351

Bond lengths

Bond angles

Torsions

Rings

Ligand G98 A 351

Bond lengths

Bond angles

Torsions

Rings
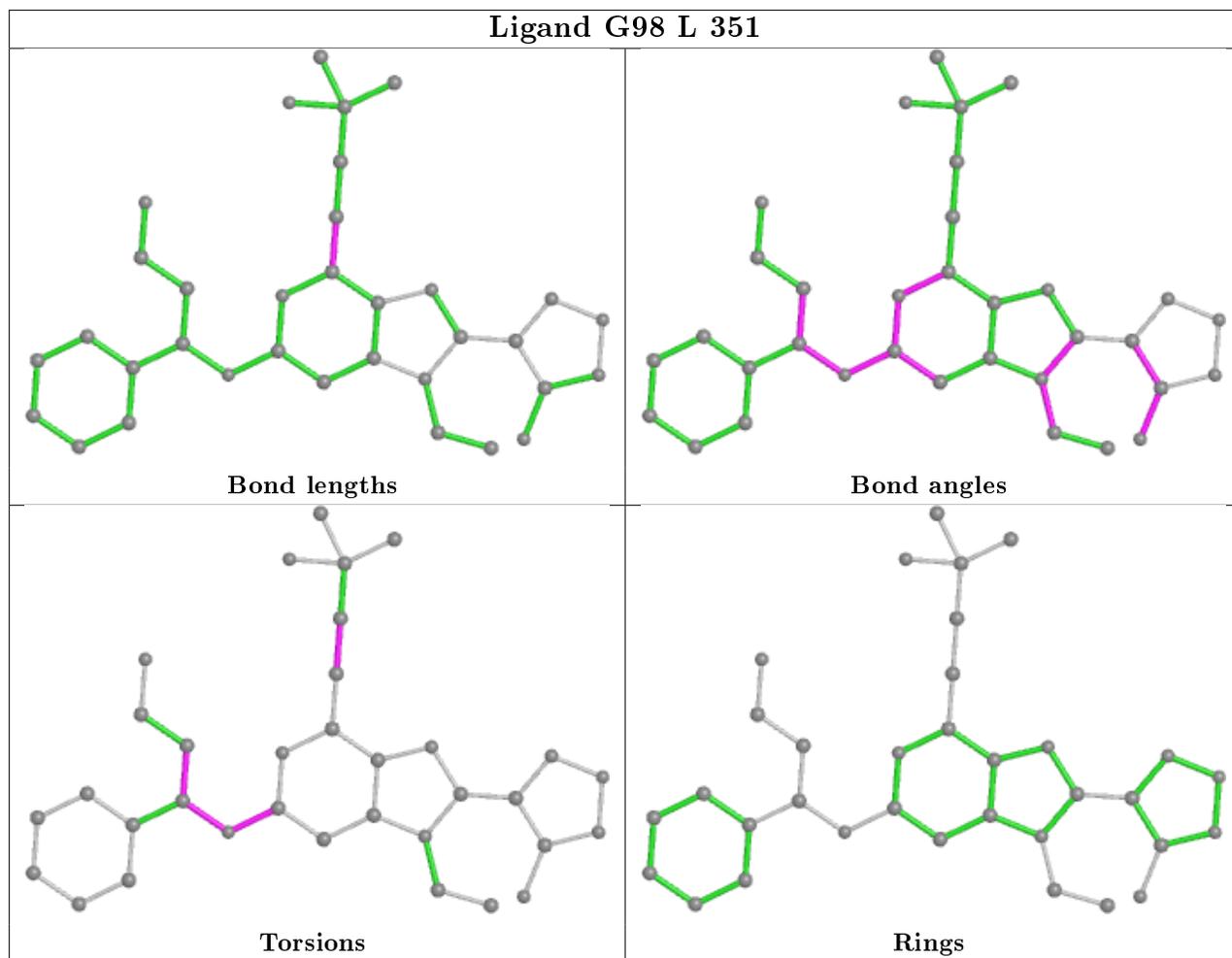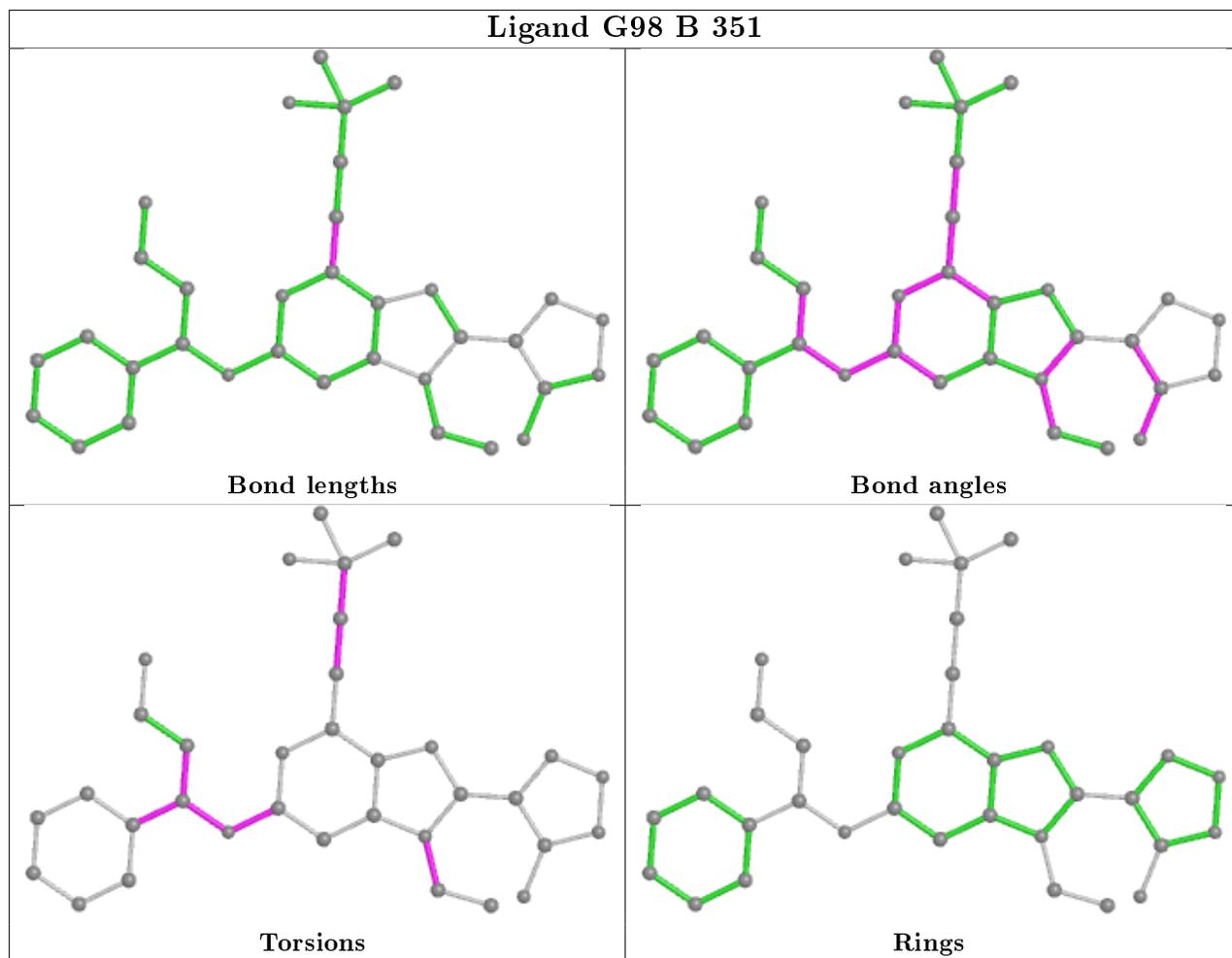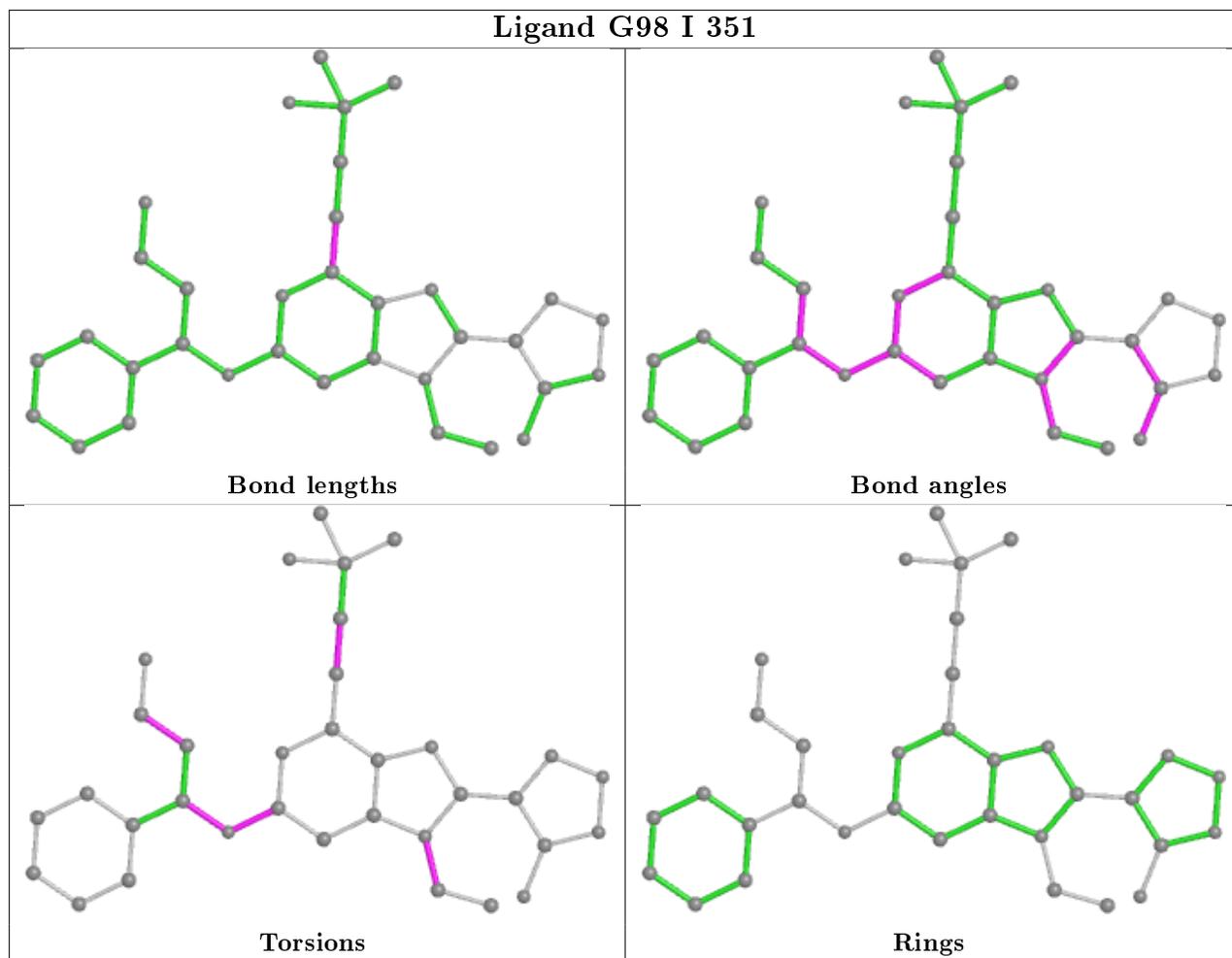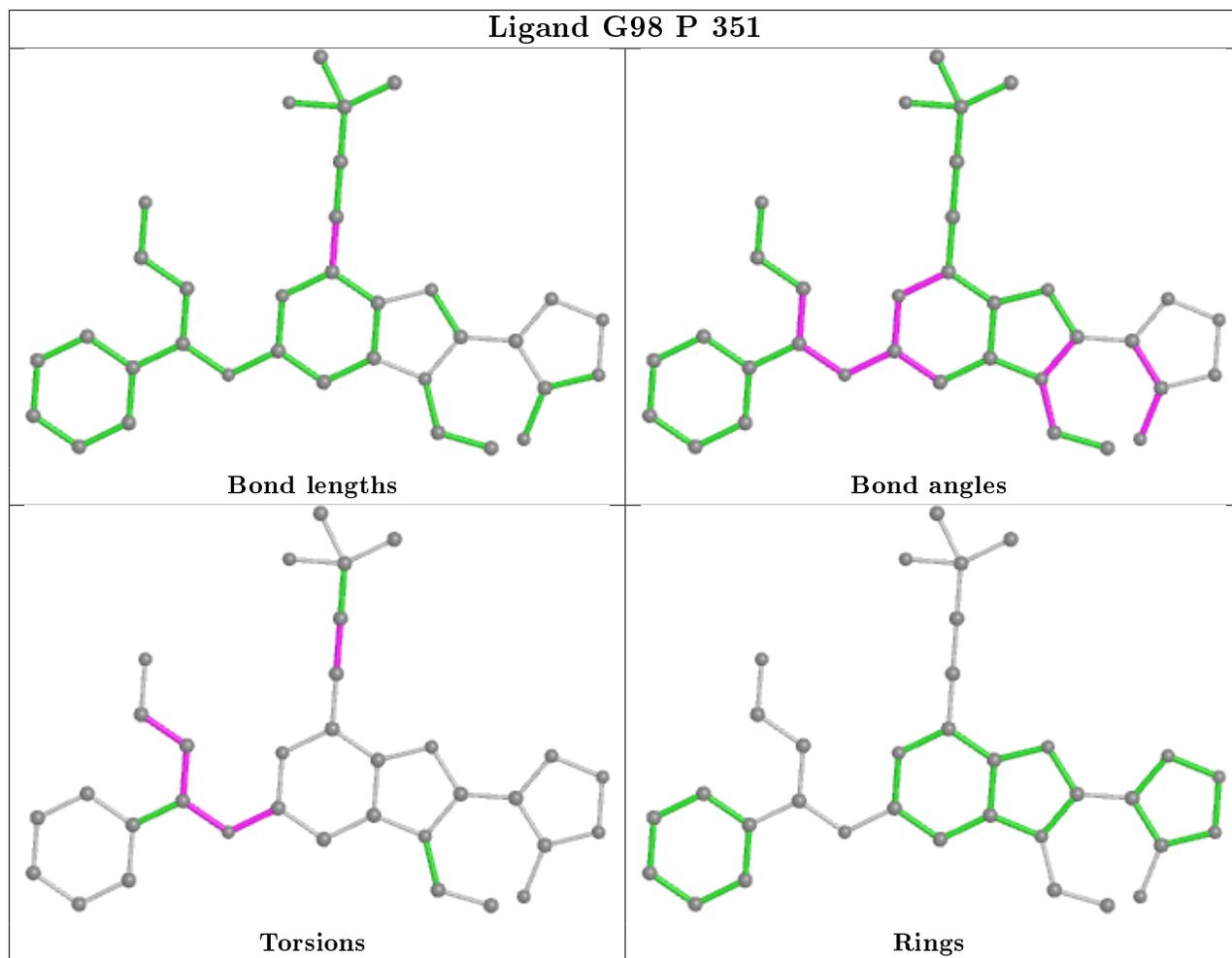
5.7 Other polymers (i)

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(Å²)	Q<0.9
1	A	341/350 (97%)	0.54	19 (5%)	24	23	28, 36, 48, 76	0
1	B	337/350 (96%)	0.59	26 (7%)	13	12	28, 36, 47, 58	0
1	E	341/350 (97%)	0.54	16 (4%)	31	30	27, 36, 46, 54	0
1	I	345/350 (98%)	0.22	12 (3%)	44	43	27, 36, 47, 55	0
1	L	336/350 (96%)	0.67	37 (11%)	5	5	26, 37, 47, 55	0
1	P	341/350 (97%)	0.59	37 (10%)	5	5	27, 37, 48, 68	0
2	C	20/20 (100%)	1.54	7 (35%)	0	0	37, 42, 53, 53	0
2	F	20/20 (100%)	0.87	3 (15%)	2	2	36, 41, 54, 54	0
2	G	20/20 (100%)	0.86	4 (20%)	1	0	39, 43, 56, 56	0
2	J	20/20 (100%)	1.30	5 (25%)	0	0	39, 42, 52, 53	0
2	N	20/20 (100%)	0.63	2 (10%)	7	6	38, 42, 55, 56	0
2	Q	20/20 (100%)	1.52	6 (30%)	0	0	39, 43, 54, 55	0
All	All	2161/2220 (97%)	0.56	174 (8%)	12	11	26, 37, 48, 76	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	34	ALA	9.4
1	L	15	VAL	9.0
2	C	5	THR	8.9
1	L	14	SER	8.0
2	Q	5	THR	7.5

## 6.2 Non-standard residues in protein, DNA, RNA chains (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
1	SEP	P	10	10/11	0.43	0.34	67,67,71,71	0
1	SEP	A	10	10/11	0.54	0.31	70,72,72,73	0
1	SEP	I	10	10/11	0.75	0.18	51,51,51,52	0
1	SEP	E	10	10/11	0.81	0.18	48,50,51,51	0
1	SEP	L	338	10/11	0.86	0.26	48,49,53,53	0
1	SEP	E	338	10/11	0.93	0.17	46,47,47,48	0
1	SEP	B	338	10/11	0.94	0.10	45,46,47,48	0
1	SEP	I	338	10/11	0.95	0.14	47,48,50,51	0
1	TPO	L	197	11/12	0.95	0.10	35,35,36,36	0
1	TPO	P	197	11/12	0.96	0.11	35,35,36,38	0
1	SEP	A	338	10/11	0.96	0.09	41,44,46,47	0
1	TPO	B	197	11/12	0.97	0.15	33,34,34,34	0
1	SEP	P	338	10/11	0.97	0.09	44,46,47,47	0
1	TPO	I	197	11/12	0.97	0.12	28,31,33,33	0
1	TPO	A	197	11/12	0.98	0.18	32,34,34,35	0
1	TPO	E	197	11/12	0.98	0.15	32,34,34,34	0

6.3 Carbohydrates (i)

There are no carbohydrates 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
3	G98	L	351	34/34	0.87	0.19	39,42,51,51	0
3	G98	B	351	34/34	0.89	0.16	25,28,37,40	0
3	G98	I	351	34/34	0.89	0.15	24,31,40,40	0
3	G98	P	351	34/34	0.89	0.16	30,33,44,46	0
3	G98	A	351	34/34	0.90	0.15	21,24,35,37	0
3	G98	E	351	34/34	0.91	0.15	17,23,35,35	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.
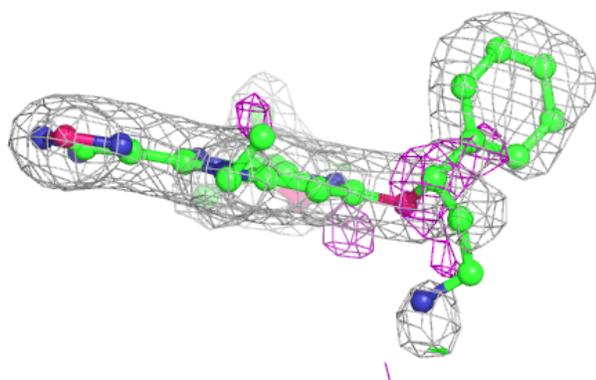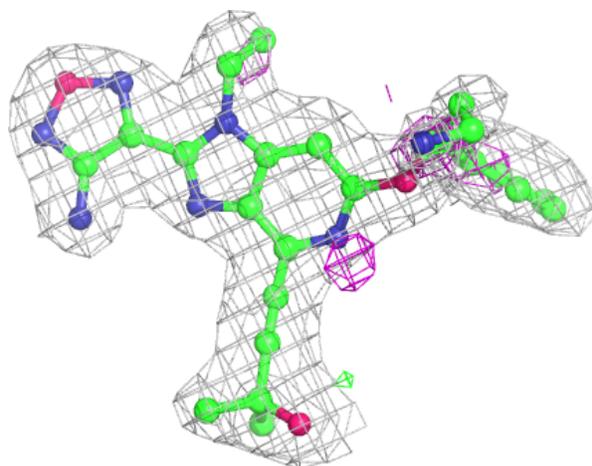
Electron density around G98 L 351:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
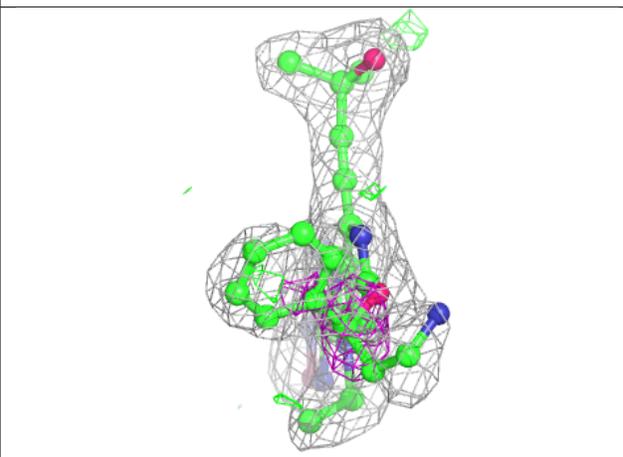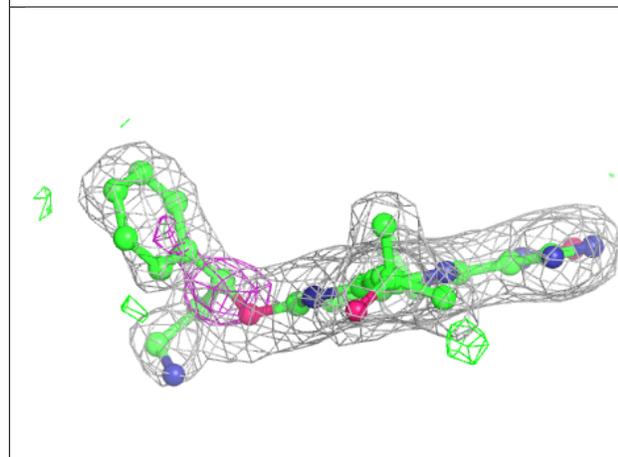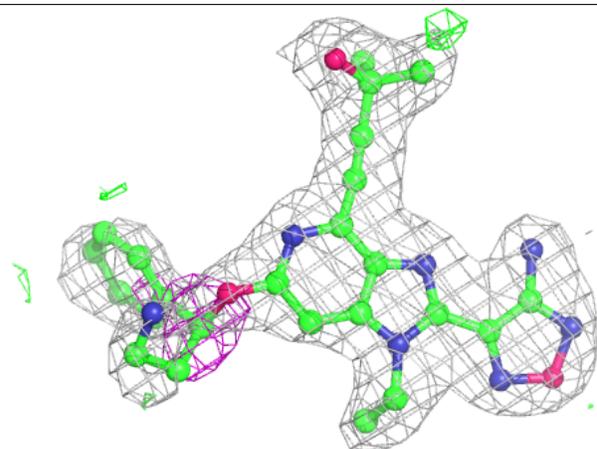and green (positive)
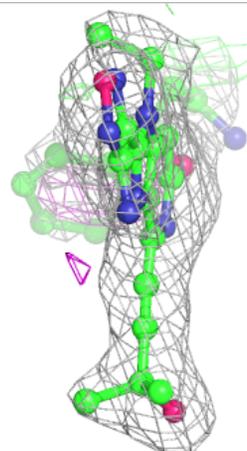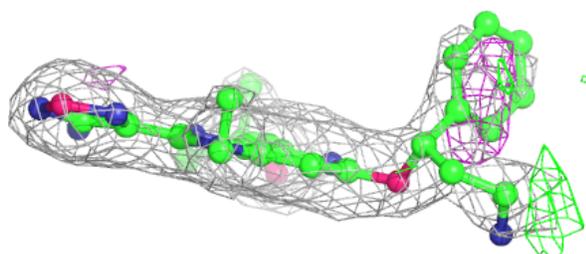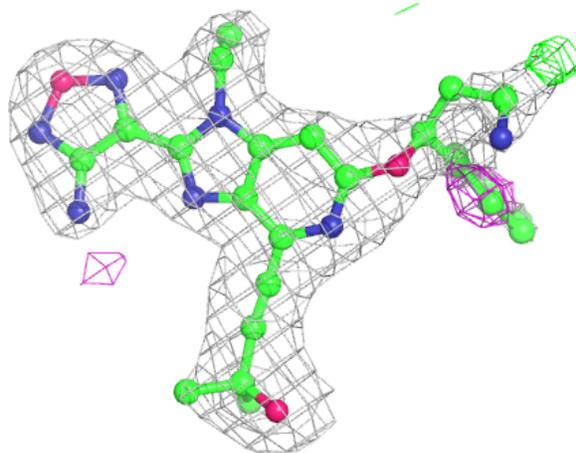
Electron density around G98 B 351:

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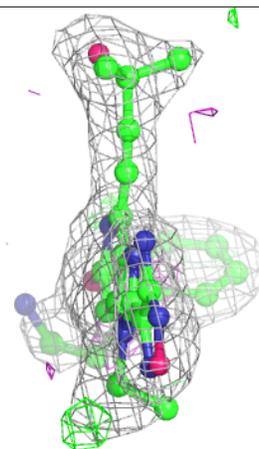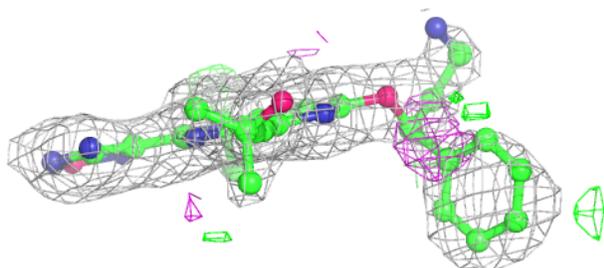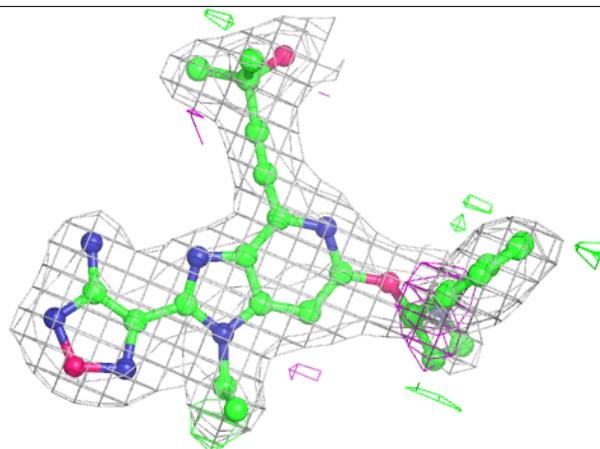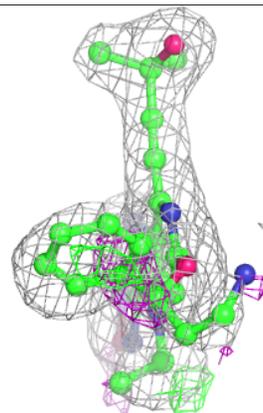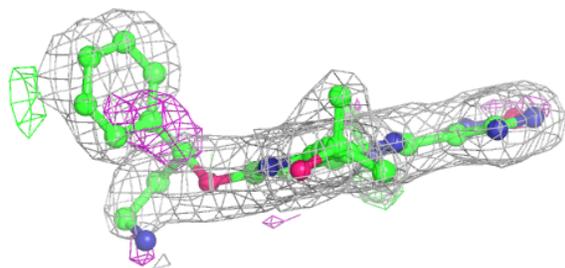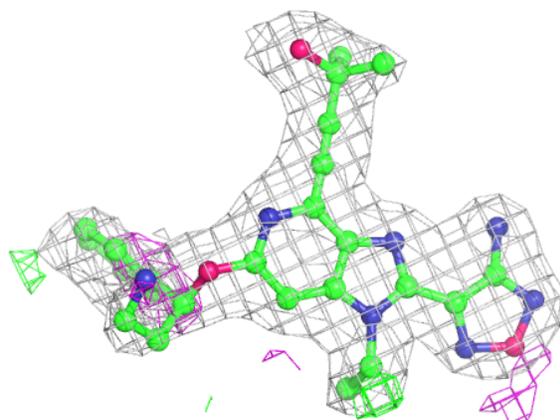mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around G98 I 351:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
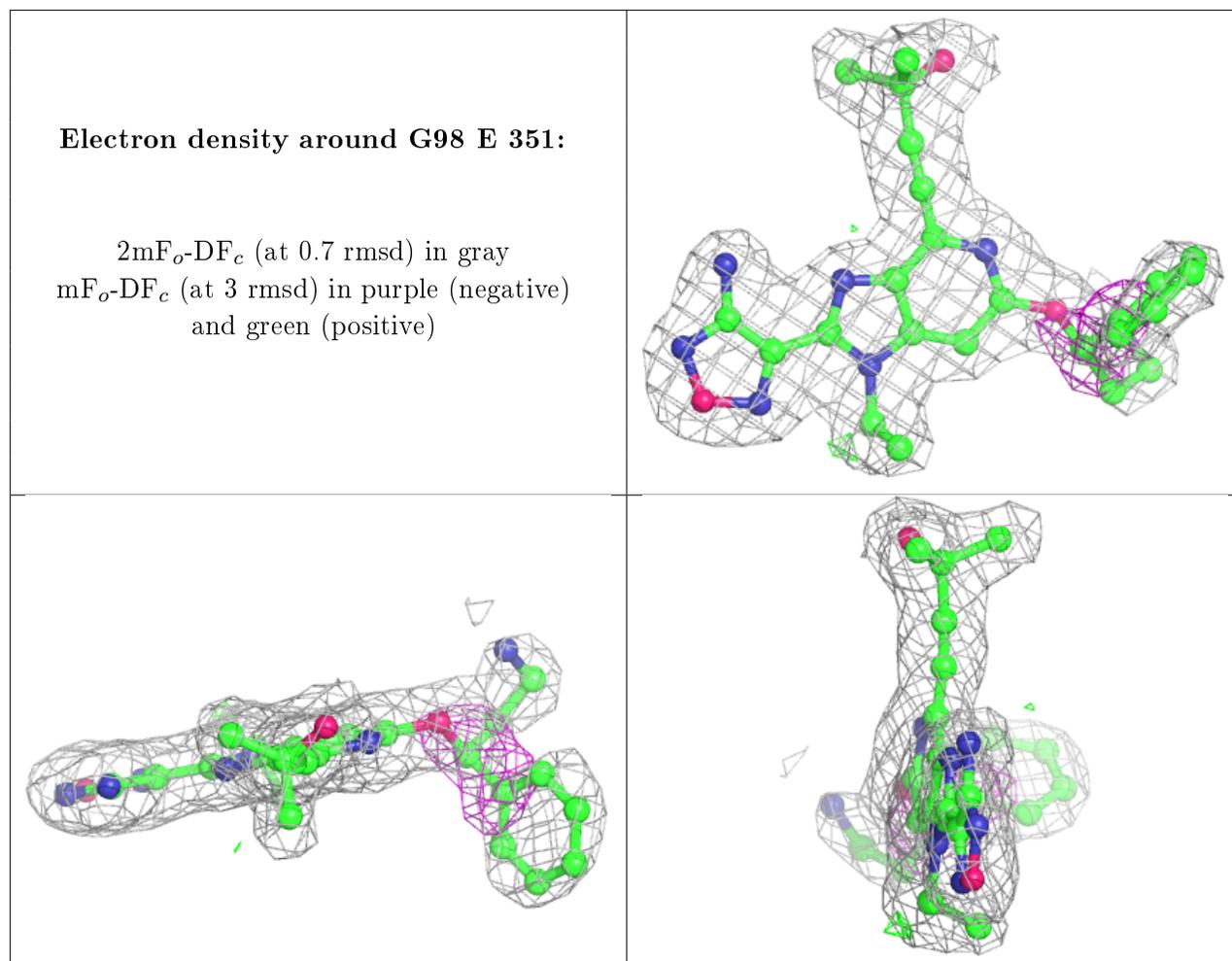
Electron density around G98 P 351:

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

Electron density around G98 A 351:

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

Electron density around G98 E 351:

$2mF_o$-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 ⓘ

There are no such residues in this entry.