WORLDWIDE PDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

May 16, 2020 – 11:56 pm BST

PDB ID : 3SKG

Title : Crystal structure of beta-site app-cleaving enzyme 1 (BACE-WT) complex with (2S)-2-((3R)-3-acetamido-3-isobutyl-2-oxo-1-pyrrolidinyl)-N-((1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-2-(1,2,3,4-tetrahydro-3-isoquinolinyl)ethyl)-4-phenylbutanamide

Authors : Muckelbauer, J.K.

Deposited on : 2011-06-22

Resolution : 2.88 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

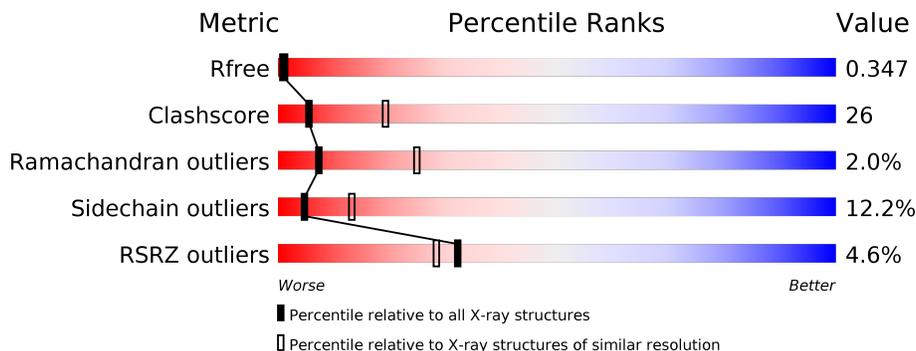|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.88 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		0.347
Clashscore		26
Ramachandran outliers		2.0%
Sidechain outliers		12.2%
RSRZ outliers		4.6%

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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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	455	3% — 44% / 35% / 6% / 15%
1	B	455	2% — 46% / 33% / 5% · / 15%
1	D	455	5% — 36% / 41% / 6% · / 15%
1	E	455	5% — 43% / 34% / 8% / 15%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12434 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	B	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	D	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			
1	E	386	Total	C	N	O	S	0	0	0
			3034	1944	503	573	14			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	EXPRESSION TAG	UNP P56817
A	-60	ALA	-	EXPRESSION TAG	UNP P56817
A	-59	SER	-	EXPRESSION TAG	UNP P56817
A	-58	MET	-	EXPRESSION TAG	UNP P56817
A	-57	THR	-	EXPRESSION TAG	UNP P56817
A	-56	GLY	-	EXPRESSION TAG	UNP P56817
A	-55	GLY	-	EXPRESSION TAG	UNP P56817
A	-54	GLN	-	EXPRESSION TAG	UNP P56817
A	-53	GLN	-	EXPRESSION TAG	UNP P56817
A	-52	MET	-	EXPRESSION TAG	UNP P56817
A	-51	GLY	-	EXPRESSION TAG	UNP P56817
A	-50	ARG	-	EXPRESSION TAG	UNP P56817
A	-49	GLY	-	EXPRESSION TAG	UNP P56817
A	-48	SER	-	EXPRESSION TAG	UNP P56817
B	-61	MET	-	EXPRESSION TAG	UNP P56817
B	-60	ALA	-	EXPRESSION TAG	UNP P56817
B	-59	SER	-	EXPRESSION TAG	UNP P56817
B	-58	MET	-	EXPRESSION TAG	UNP P56817
B	-57	THR	-	EXPRESSION TAG	UNP P56817
B	-56	GLY	-	EXPRESSION TAG	UNP P56817
B	-55	GLY	-	EXPRESSION TAG	UNP P56817

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-54	GLN	-	EXPRESSION TAG	UNP P56817
B	-53	GLN	-	EXPRESSION TAG	UNP P56817
B	-52	MET	-	EXPRESSION TAG	UNP P56817
B	-51	GLY	-	EXPRESSION TAG	UNP P56817
B	-50	ARG	-	EXPRESSION TAG	UNP P56817
B	-49	GLY	-	EXPRESSION TAG	UNP P56817
B	-48	SER	-	EXPRESSION TAG	UNP P56817
D	-61	MET	-	EXPRESSION TAG	UNP P56817
D	-60	ALA	-	EXPRESSION TAG	UNP P56817
D	-59	SER	-	EXPRESSION TAG	UNP P56817
D	-58	MET	-	EXPRESSION TAG	UNP P56817
D	-57	THR	-	EXPRESSION TAG	UNP P56817
D	-56	GLY	-	EXPRESSION TAG	UNP P56817
D	-55	GLY	-	EXPRESSION TAG	UNP P56817
D	-54	GLN	-	EXPRESSION TAG	UNP P56817
D	-53	GLN	-	EXPRESSION TAG	UNP P56817
D	-52	MET	-	EXPRESSION TAG	UNP P56817
D	-51	GLY	-	EXPRESSION TAG	UNP P56817
D	-50	ARG	-	EXPRESSION TAG	UNP P56817
D	-49	GLY	-	EXPRESSION TAG	UNP P56817
D	-48	SER	-	EXPRESSION TAG	UNP P56817
E	-61	MET	-	EXPRESSION TAG	UNP P56817
E	-60	ALA	-	EXPRESSION TAG	UNP P56817
E	-59	SER	-	EXPRESSION TAG	UNP P56817
E	-58	MET	-	EXPRESSION TAG	UNP P56817
E	-57	THR	-	EXPRESSION TAG	UNP P56817
E	-56	GLY	-	EXPRESSION TAG	UNP P56817
E	-55	GLY	-	EXPRESSION TAG	UNP P56817
E	-54	GLN	-	EXPRESSION TAG	UNP P56817
E	-53	GLN	-	EXPRESSION TAG	UNP P56817
E	-52	MET	-	EXPRESSION TAG	UNP P56817
E	-51	GLY	-	EXPRESSION TAG	UNP P56817
E	-50	ARG	-	EXPRESSION TAG	UNP P56817
E	-49	GLY	-	EXPRESSION TAG	UNP P56817
E	-48	SER	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is (2S)-2-[(3R)-3-(acetylamino)-3-(2-methylpropyl)-2-oxopyrrolidin-1-yl]-N-{(1R,2S)-3-(3,5-difluorophenyl)-1-hydroxy-1-[(3R)-1,2,3,4-tetrahydroisoquinolin-3-yl]propan-2-yl}-4-phenylbutanamide (three-letter code: PB8) (formula: $C_{38}H_{46}F_2N_4O_4$).
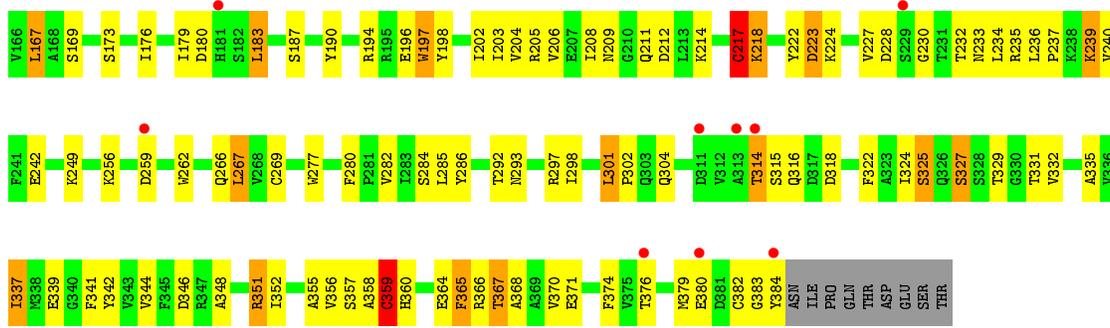
PB8
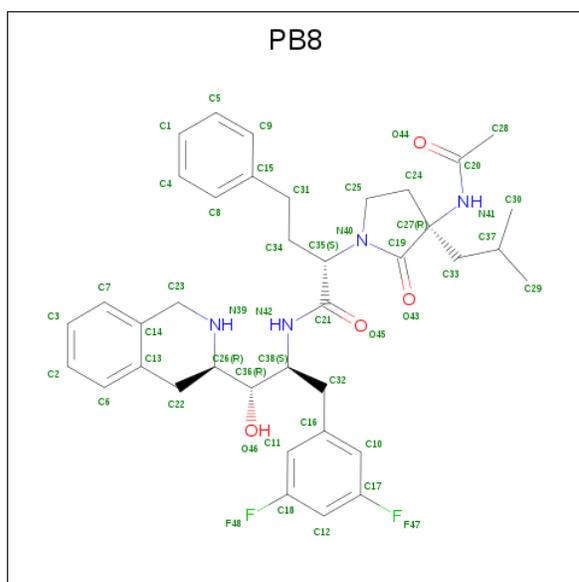
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 48	C 38	F 2	N 4	O 4	0	0
2	B	1	Total 48	C 38	F 2	N 4	O 4	0	0
2	D	1	Total 48	C 38	F 2	N 4	O 4	0	0
2	E	1	Total 48	C 38	F 2	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total 24	O 24	0	0
3	B	38	Total 38	O 38	0	0
3	D	20	Total 20	O 20	0	0
3	E	24	Total 24	O 24	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: Beta-secretase 1

- Molecule 1: Beta-secretase 1

• Molecule 1: Beta-secretase 1

Chain D:

• Molecule 1: Beta-secretase 1

Chain E:

4　Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.24Å　　130.45Å　　86.87Å 90.00°　　96.65°　　90.00°	Depositor
Resolution (Å)	30.63　−　2.88 30.63　−　2.88	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.63-2.88) 98.9 (30.63-2.88)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.48 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.255　,　0.348 0.256　,　0.347	Depositor DCC
R_{free} test set	2159 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.1	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.9	EDS
L-test for twinning[2]	$<|L|> = 0.47, <L^2> = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	12434	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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 22.23 % 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 5.9537e-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: PB8

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	1.37	7/3112 (0.2%)	1.21	10/4232 (0.2%)
1	B	1.39	12/3112 (0.4%)	1.24	15/4232 (0.4%)
1	D	1.38	8/3112 (0.3%)	1.22	11/4232 (0.3%)
1	E	1.39	7/3112 (0.2%)	1.26	21/4232 (0.5%)
All	All	1.38	34/12448 (0.3%)	1.23	57/16928 (0.3%)

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	D	0	1

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	CYS	CB-SG	-14.77	1.57	1.82
1	E	217	CYS	CB-SG	-11.38	1.62	1.82
1	B	359	CYS	CB-SG	-11.33	1.62	1.82
1	B	364	GLU	CG-CD	9.12	1.65	1.51
1	A	364	GLU	CG-CD	9.08	1.65	1.51

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	CYS	CA-CB-SG	-10.02	95.96	114.00
1	E	235	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	B	96	ARG	NE-CZ-NH2	-9.77	115.42	120.30
1	E	235	ARG	NE-CZ-NH1	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	217	CYS	CA-CB-SG	-8.92	97.95	114.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	197	TRP	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	3034	0	2948	147	0
1	B	3034	0	2948	127	0
1	D	3034	0	2950	188	0
1	E	3034	0	2948	156	0
2	A	48	0	46	9	0
2	B	48	0	46	7	0
2	D	48	0	46	5	0
2	E	48	0	46	10	0
3	A	24	0	0	7	0
3	B	38	0	0	2	0
3	D	20	0	0	2	0
3	E	24	0	0	3	0
All	All	12434	0	11978	629	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 26.

The worst 5 of 629 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:A:73:GLN:HG2	3:A:414:HOH:O	1.43	1.18
1:D:376:THR:HA	3:D:412:HOH:O	1.53	1.07
1:E:63:LEU:HD12	1:E:80:LEU:HB3	1.34	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:394:PB8:H28A	2:E:394:PB8:H31A	1.30	1.07
2:E:394:PB8:H28A	2:E:394:PB8:C31	1.88	1.01

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	384/455 (84%)	338 (88%)	39 (10%)	7 (2%)	8	27
1	B	384/455 (84%)	338 (88%)	42 (11%)	4 (1%)	15	42
1	D	384/455 (84%)	336 (88%)	37 (10%)	11 (3%)	4	16
1	E	384/455 (84%)	337 (88%)	38 (10%)	9 (2%)	6	21
All	All	1536/1820 (84%)	1349 (88%)	156 (10%)	31 (2%)	7	25

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	107	LYS
1	D	55	GLN
1	D	92	ASN
1	D	380	GLU

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	329/381 (86%)	294 (89%)	35 (11%)	6	19
1	B	329/381 (86%)	290 (88%)	39 (12%)	5	14
1	D	329/381 (86%)	282 (86%)	47 (14%)	3	9
1	E	329/381 (86%)	289 (88%)	40 (12%)	5	13
All	All	1316/1524 (86%)	1155 (88%)	161 (12%)	5	13

5 of 161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	359	CYS
1	D	185	THR
1	E	301	LEU
1	D	9	LYS
1	D	94	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	143	GLN
1	B	153	GLN
1	B	360	HIS
1	A	271	GLN
1	B	211	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	PB8	E	394	-	52,52,52	1.92	15 (28%)	60,74,74	2.93	28 (46%)
2	PB8	D	394	-	52,52,52	2.15	12 (23%)	60,74,74	2.93	28 (46%)
2	PB8	A	394	-	52,52,52	2.19	12 (23%)	60,74,74	2.48	22 (36%)
2	PB8	B	394	-	52,52,52	2.00	13 (25%)	60,74,74	2.92	26 (43%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PB8	E	394	-	-	14/39/64/64	0/5/5/5
2	PB8	D	394	-	-	6/39/64/64	0/5/5/5
2	PB8	A	394	-	-	6/39/64/64	0/5/5/5
2	PB8	B	394	-	-	18/39/64/64	0/5/5/5

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	394	PB8	C7-C14	7.55	1.52	1.39
2	E	394	PB8	C27-C19	-5.84	1.47	1.52
2	D	394	PB8	C14-C13	-5.58	1.29	1.40
2	B	394	PB8	C6-C13	5.54	1.49	1.39
2	D	394	PB8	C27-C19	-5.54	1.47	1.52

The worst 5 of 104 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	394	PB8	O43-C19-C27	-10.17	118.06	126.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	394	PB8	C25-N40-C19	-9.77	107.14	113.43
2	B	394	PB8	C28-C20-N41	9.24	127.95	115.98
2	E	394	PB8	O43-C19-C27	-8.71	119.30	126.67
2	E	394	PB8	C16-C10-C17	8.27	126.33	118.81

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	394	PB8	C28-C20-N41-C27
2	E	394	PB8	O44-C20-N41-C27
2	E	394	PB8	C19-C27-C33-C37
2	E	394	PB8	C24-C27-C33-C37
2	E	394	PB8	C31-C34-C35-N40

There are no ring outliers.

4 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	394	PB8	10	0
2	D	394	PB8	5	0
2	A	394	PB8	9	0
2	B	394	PB8	7	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 PB8 E 394

Bond lengths

Bond angles

Torsions

Rings

Ligand PB8 D 394

Bond lengths

Bond angles

Torsions

Rings

Ligand PB8 A 394

Bond lengths

Bond angles

Torsions

Rings

Ligand PB8 B 394

Bond lengths

Bond angles

Torsions

Rings
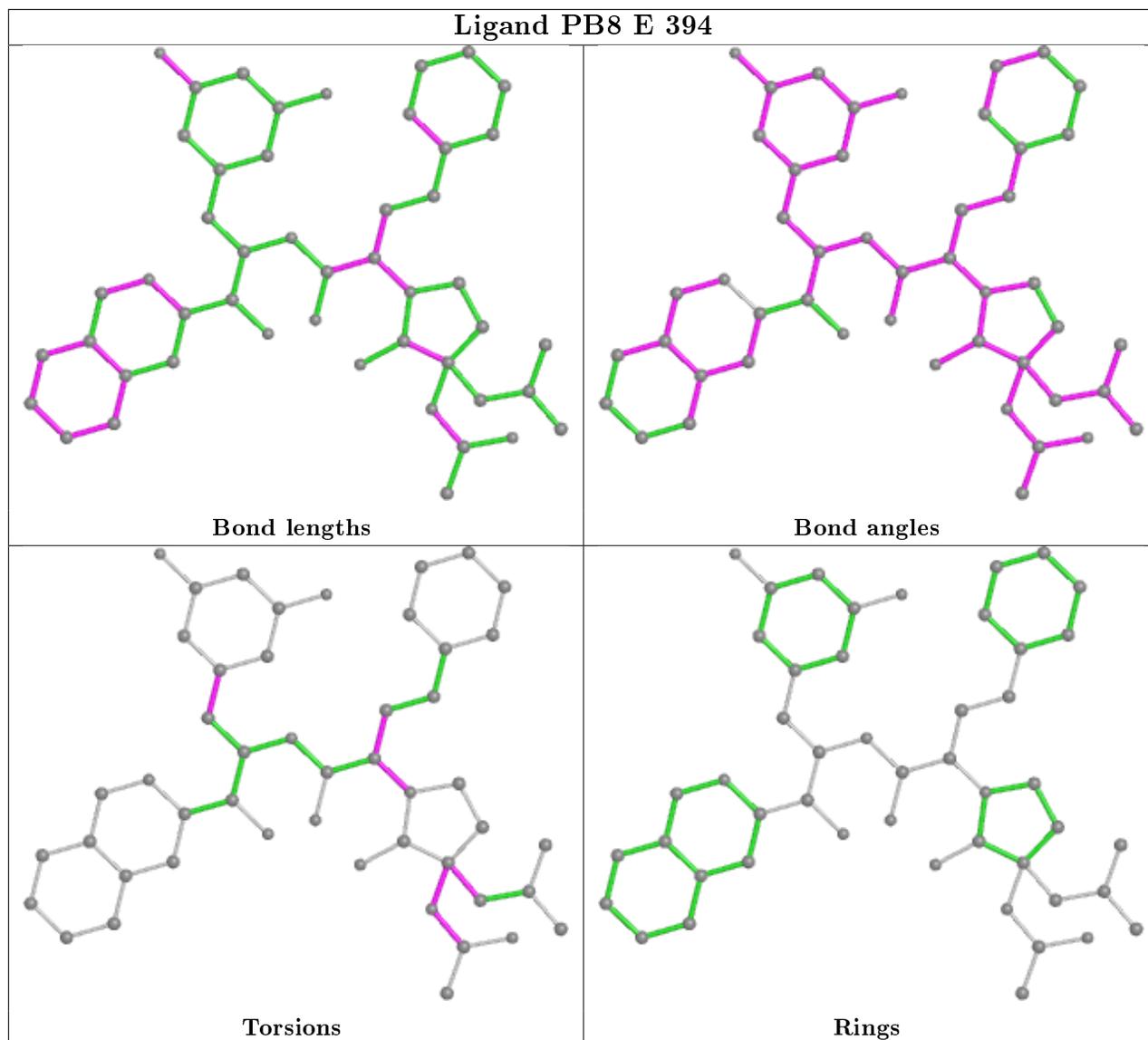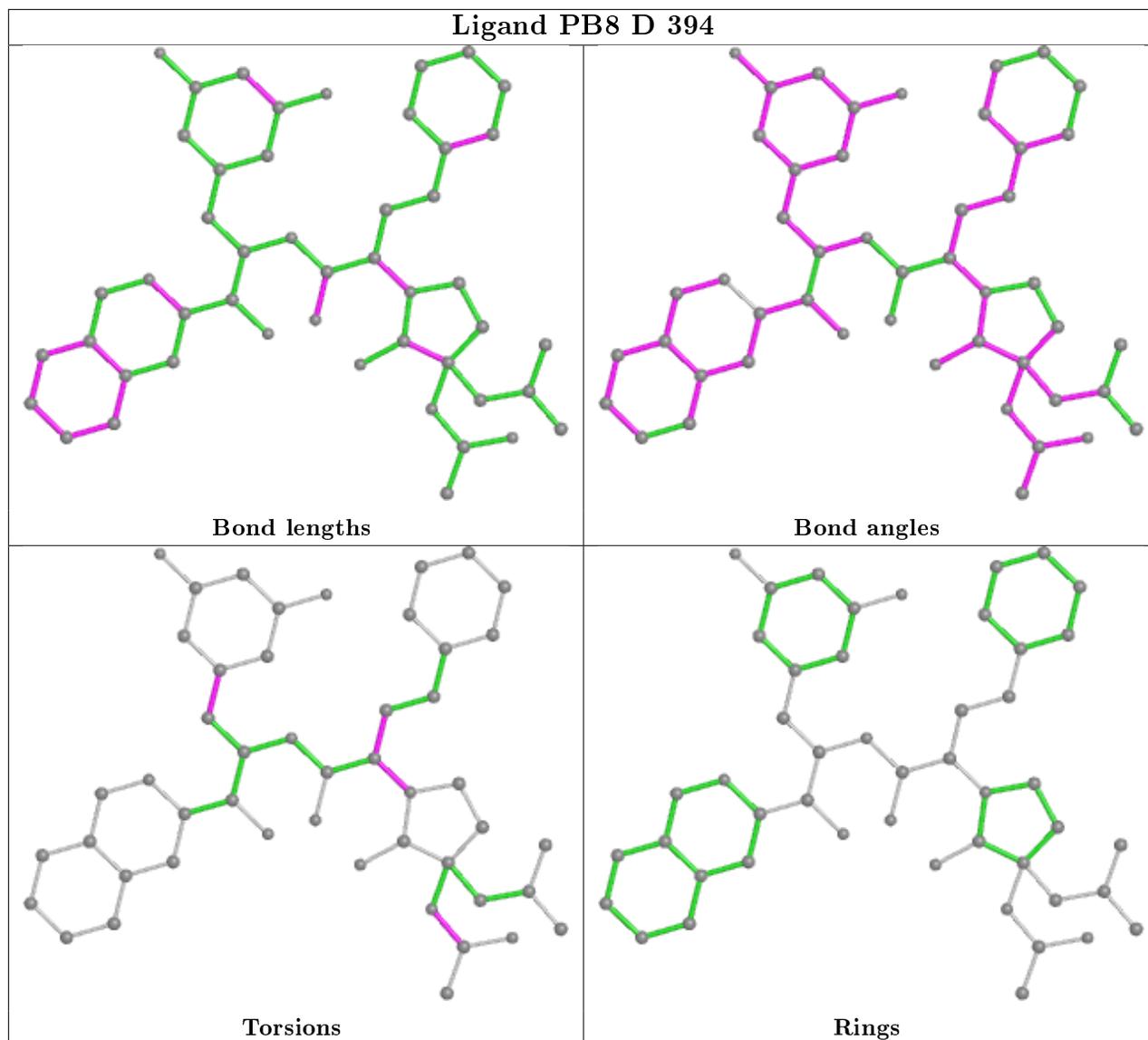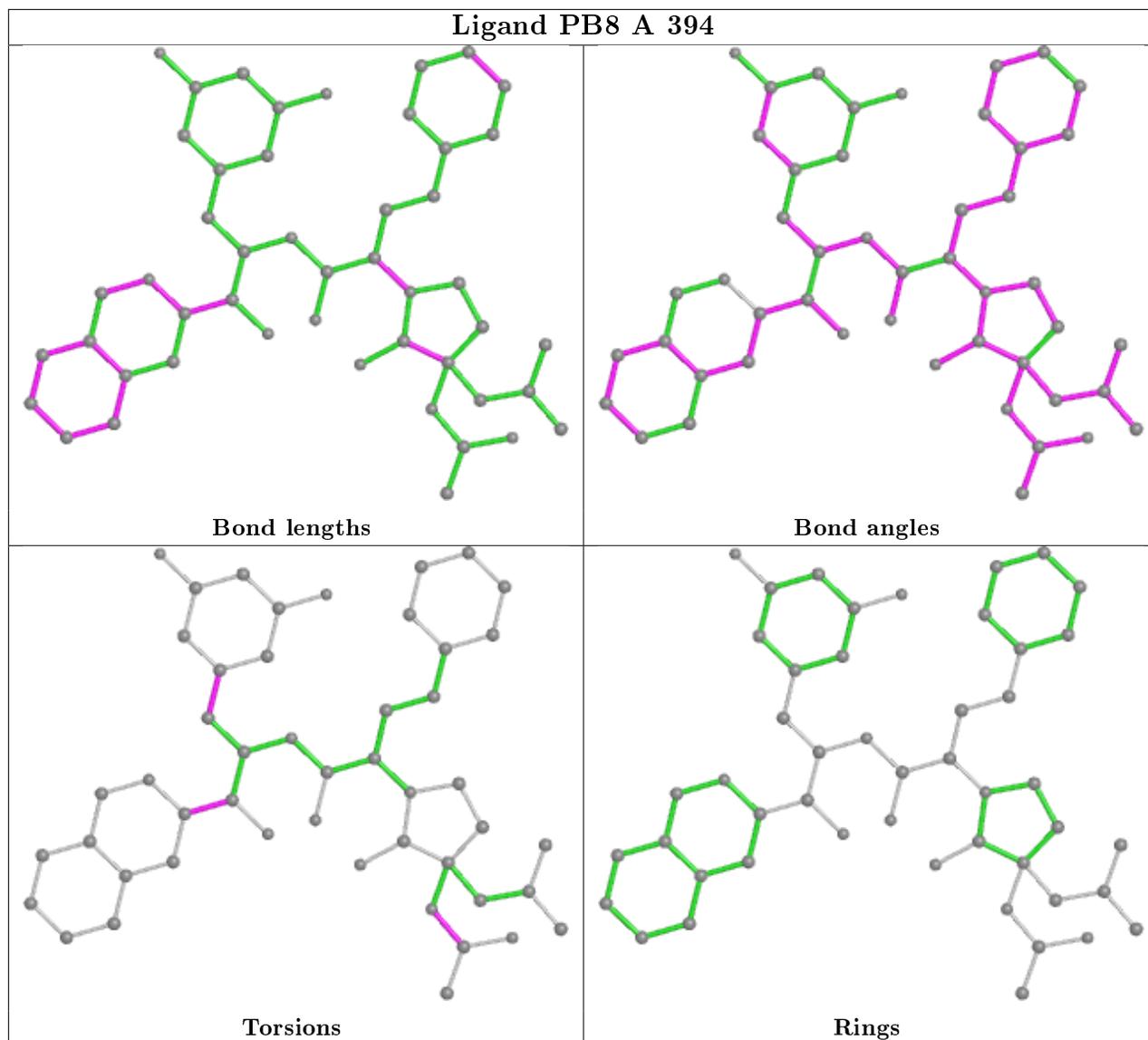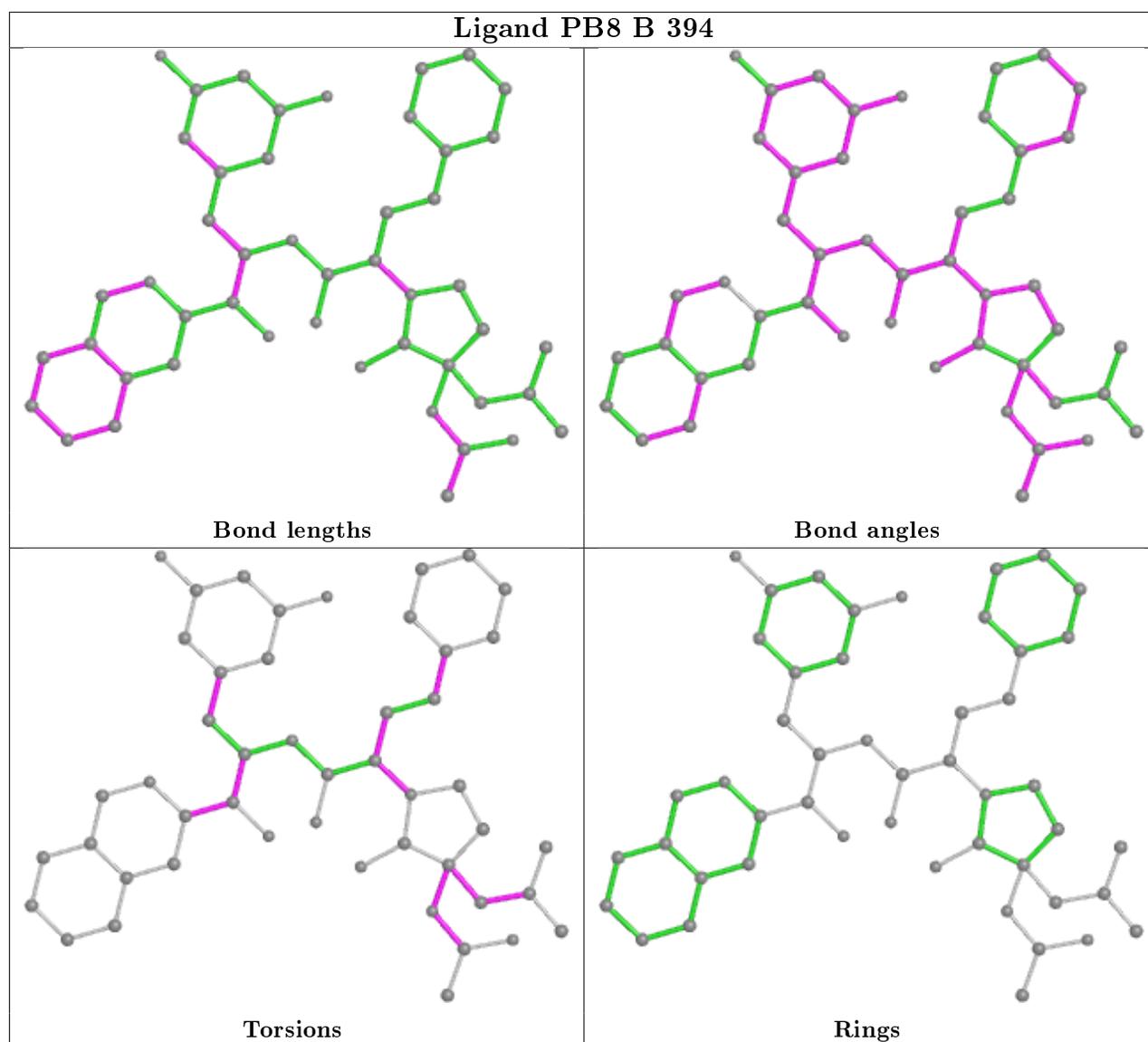
5.7 Other polymers (i)

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 ⓘ

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	386/455 (84%)	0.17	12 (3%)	49	45	4, 18, 36, 59	0
1	B	386/455 (84%)	0.12	11 (2%)	53	50	3, 16, 35, 47	0
1	D	386/455 (84%)	0.45	24 (6%)	20	16	10, 24, 39, 59	0
1	E	386/455 (84%)	0.42	24 (6%)	20	16	10, 23, 41, 57	0
All	All	1544/1820 (84%)	0.29	71 (4%)	32	28	3, 20, 38, 59	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	THR	5.7
1	E	378	ASP	4.8
1	E	311	ASP	4.8
1	B	313	ALA	4.6
1	A	376	THR	4.0

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

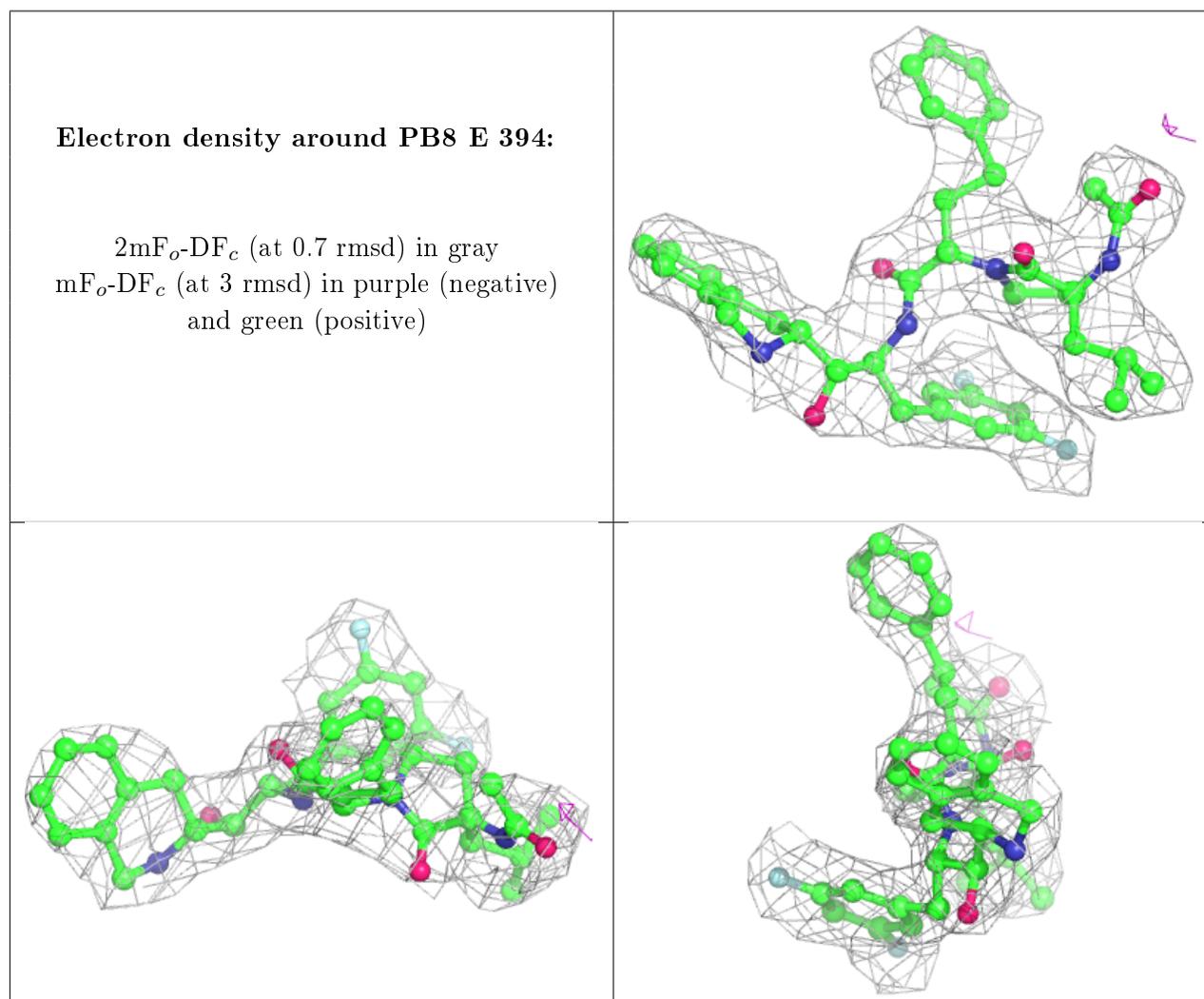There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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($\mathrm{\AA}^2$)	Q<0.9
2	PB8	E	394	48/48	0.91	0.21	6,15,20,22	0
2	PB8	D	394	48/48	0.93	0.18	3,15,24,25	0
2	PB8	B	394	48/48	0.93	0.19	3,10,15,20	0
2	PB8	A	394	48/48	0.94	0.19	2,11,21,24	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.
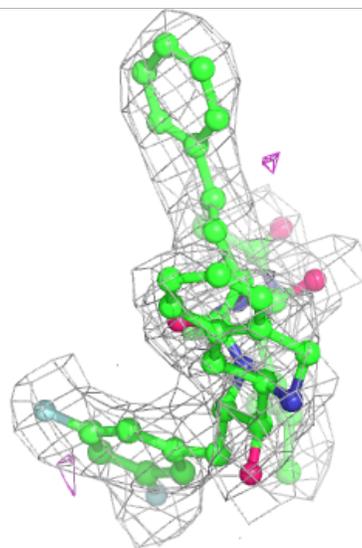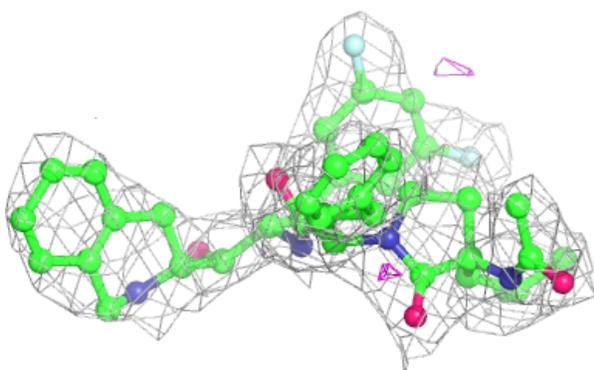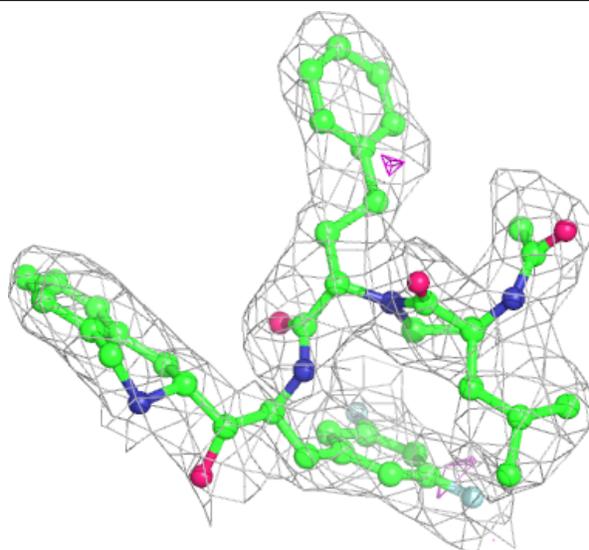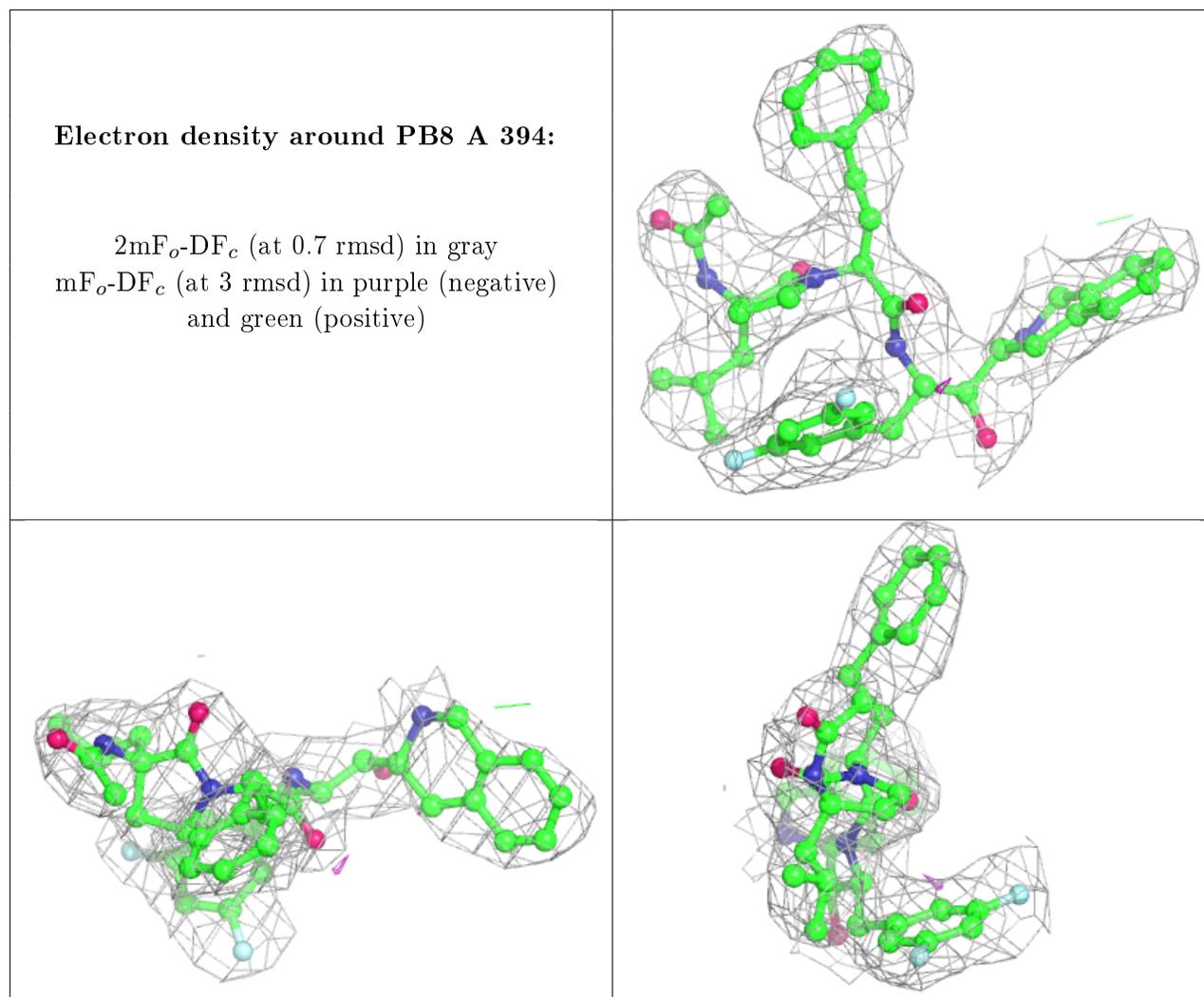
Electron density around PB8 E 394:

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

Electron density around PB8 D 394:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
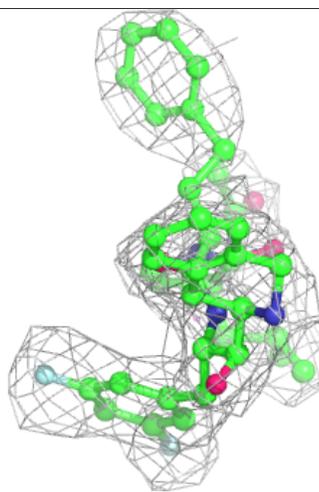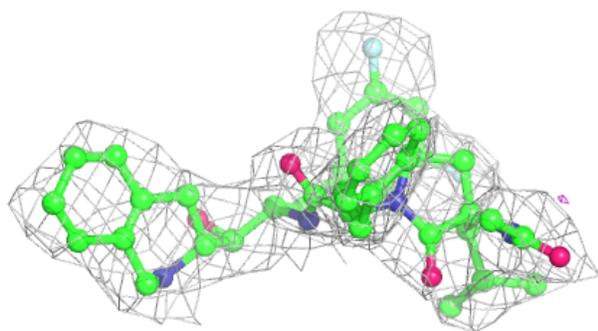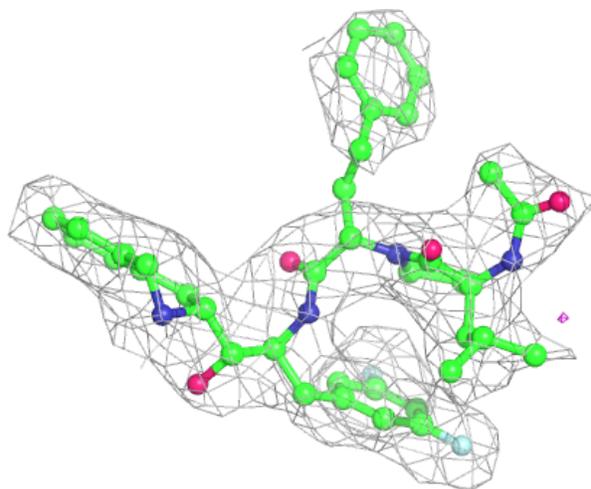
Electron density around PB8 B 394:

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

Electron density around PB8 A 394:

$2mF_o$-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.