



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 01:55 AM EST

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-pyrrolidiny1)-N-((1S,2R)-1-(3,5-difluorobenzyl)-2-hydroxy-2-(1,2,3,4-tetrahydro-3-isoquinoliny1)ethyl)-4-phenylbutanamide
Authors : Muckelbauer, J.K.
Deposited on : 2011-06-22
Resolution : 2.88 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

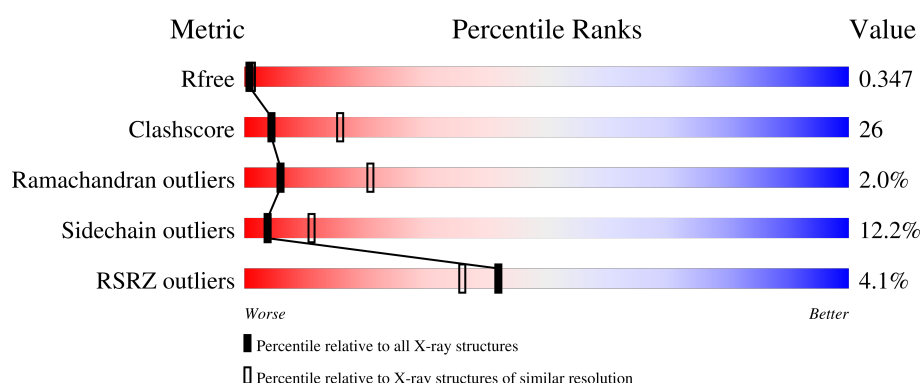
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (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 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	455	<div> <div>3%</div> <div> <div>44%</div> <div>35%</div> <div>6%</div> <div>15%</div> </div> </div>
1	B	455	<div> <div>2%</div> <div> <div>46%</div> <div>33%</div> <div>5%</div> <div>15%</div> </div> </div>
1	D	455	<div> <div>4%</div> <div> <div>36%</div> <div>41%</div> <div>6%</div> <div>15%</div> </div> </div>
1	E	455	<div> <div>5%</div> <div> <div>43%</div> <div>34%</div> <div>8%</div> <div>15%</div> </div> </div>

2 Entry composition

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:

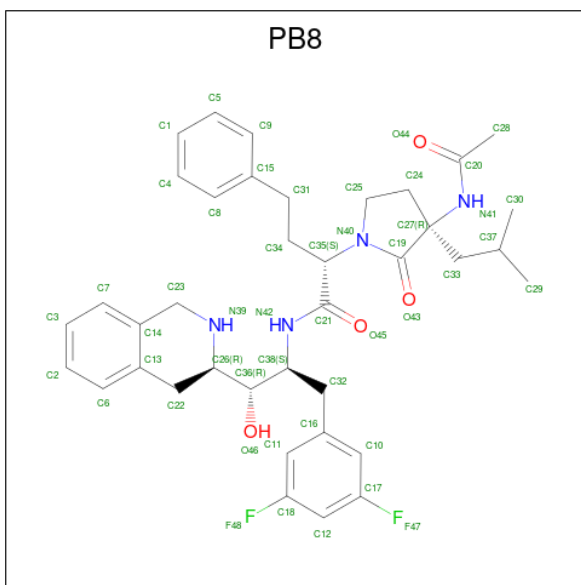
Chain	Residue	Modelled	Actual	Comment	Reference
A	-61	MET	-	expression tag	UNP P56817
A	-60	ALA	-	expression tag	UNP P56817
A	-59	SER	-	expression tag	UNP P56817
A	-58	MET	-	expression tag	UNP P56817
A	-57	THR	-	expression tag	UNP P56817
A	-56	GLY	-	expression tag	UNP P56817
A	-55	GLY	-	expression tag	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: C₃₈H₄₆F₂N₄O₄).



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	O	0	0
			24	24		
3	B	38	Total	O	0	0
			38	38		
3	D	20	Total	O	0	0
			20	20		
3	E	24	Total	O	0	0
			24	24		

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.

Chain A:

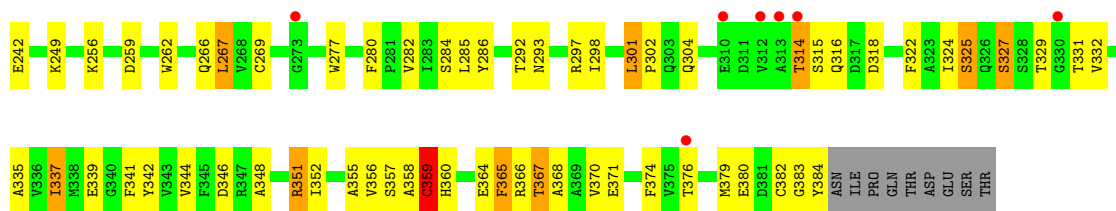
3% 44% 35% 6% 15%

Met	ALA	SER	THR	GLY	GLN	GLN	MET	MET	GLY	ARG	GLY	SER	ALA	VAL	LEU	PRO	ALA	HIS	GLY	THR	GLN	HIS	GLY	ILE	ARG	LEU	PRO	LEU	ARG	SER	GLY	LEU	GLY	GLY	ALA	PRO	LEU	LEU	ARG	LEU	PRO	GLU	THR	ASP	GLU	GLU	PRO	GLU	PRO	GLY	ARG	GLY	THR	PRO
F-1	V0	E1	N2	V3	D4	K9	S10	A97	G11	Y14	Y15	E17	V20	G21	S22	Q25	T26	L27	N28	D32	F38	A39	V40	G41	H45	P46	F47	L48	V51	V52	G53	B54	Q55	L56	S57	V60	R61	D62	L63	V67	Q73	G74	K75	W76	E77	L80								
D83	L84	P88	H89	G90	P91	A96	R97	A97	N98	E104	K107	N111	W115	I118	L119	G120	L121	A122	Y123	D130	D131	S132	L133	F137	L140	V141	H144	T145	N148	L149	F150	Q153	L154	C155	G156	A157	G158	F159	P160	L161	N162	Q163	S164	V165	L167	A168								
S169	V170	M174	I175	I176	G177	G178	W189	Y190	I193	R194	R195	E196	W197	Y198	Y199	E200	R205	S284	V206	E207	I208	M209	G210	Q211	D212	L213	C217	K218	N221	Q223	K224	S225	L226	V227	D228	S229	T231	S315	Q316	D317	D318	K321	F322	A323	I324	S325	Q326	S327	S328	S247	T329	C330		
K249	A250	A251	S252	G260	F261	W262	E265	Q266	L267	W277	N278	I279	F280	P281	W282	I283	A355	V356	S357	A358	C359	D363	E364	T367	V375	T376	L377	S378	M379	E380	D381	Y384	ASN	ILE	PRO	GLN	THR	ASP	GLU	SER	THR													

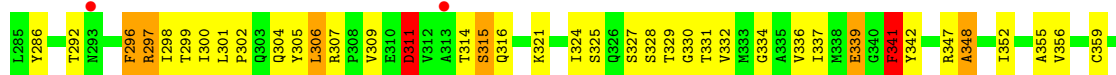
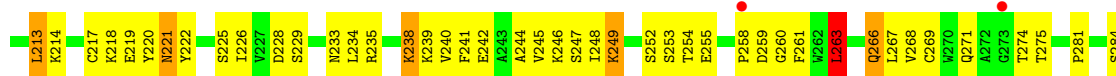
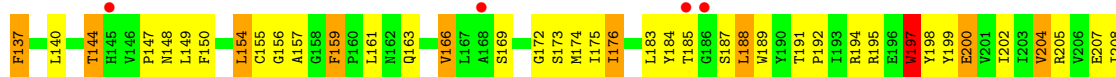
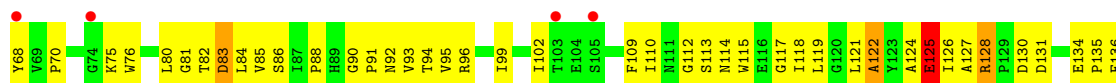
Chain B:

2% 46% 33% 5% 15%

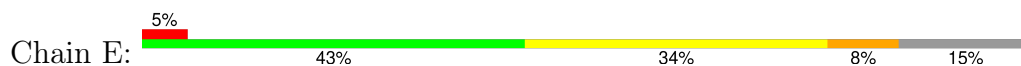
MET
ALA
SER
MET
THR
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GLY
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GLN
MET
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ARG
GLY
SER
ALA
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VAL
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PRO
HIS
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THR
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PRO
LEU
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GLY
LEU
GLY
ALA
PRO
LEU
GLY
GLY
R50
R54
R55
R56
T59
Y60
L63
Y68
V69
P70
Q73
R74
R75
R76
E77
L80
R81
R82
D83
L84
S86
I87
G90
P91
N92
N93
T94
Y95
R96
I102
S105
D106
I110
E116
G117
I118
L119
A124
E125
R126
A127
P128
D129
D130
D131
S132
L133
E134
P135
F136
F137
D138
S139
L140
V141
K142
Q143
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L149
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N233
L234
R235
L236
P237
K238
K239
V240
S241

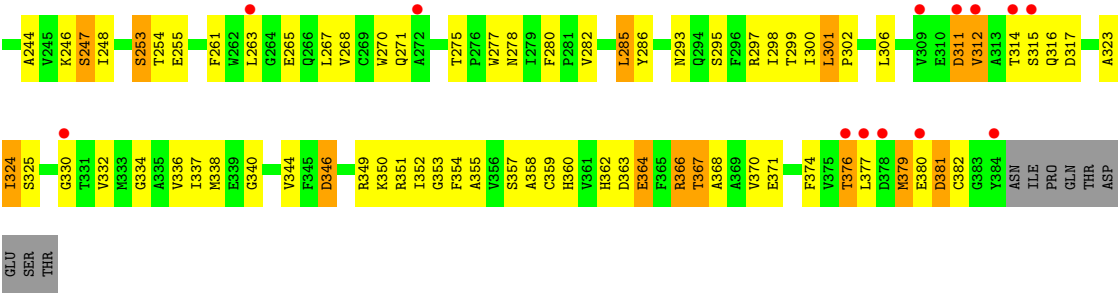


• Molecule 1: Beta-secretase 1



• Molecule 1: Beta-secretase 1





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.38 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.029 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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(°)	Ideal(°)
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:H31A	2:E:394:PB8:H28A	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%)	7	23
1	B	384/455 (84%)	338 (88%)	42 (11%)	4 (1%)	13	36
1	D	384/455 (84%)	336 (88%)	37 (10%)	11 (3%)	3	13
1	E	384/455 (84%)	337 (88%)	38 (10%)	9 (2%)	5	18
All	All	1536/1820 (84%)	1349 (88%)	156 (10%)	31 (2%)	6	21

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%)	5	16
1	B	329/381 (86%)	290 (88%)	39 (12%)	4	12
1	D	329/381 (86%)	282 (86%)	47 (14%)	2	7
1	E	329/381 (86%)	289 (88%)	40 (12%)	4	11
All	All	1316/1524 (86%)	1155 (88%)	161 (12%)	4	11

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

Mol	Chain	Res	Type
1	D	341	PHE
1	E	239	LYS
1	D	375	VAL
1	E	87	ILE
1	E	314	THR

Sometimes 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	360	HIS
1	D	37	ASN
1	D	111	ASN
1	A	271	GLN
1	B	143	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 oligosaccharides in this entry.

5.6 Ligand geometry

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	D	394	-	52,52,52	2.29	12 (23%)	58,74,74	3.00	28 (48%)
2	PB8	B	394	-	52,52,52	2.14	13 (25%)	58,74,74	3.06	27 (46%)
2	PB8	E	394	-	52,52,52	2.04	15 (28%)	58,74,74	2.97	26 (44%)
2	PB8	A	394	-	52,52,52	2.31	15 (28%)	58,74,74	2.63	22 (37%)

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	D	394	-	-	7/39/64/64	0/5/5/5
2	PB8	B	394	-	-	18/39/64/64	0/5/5/5
2	PB8	E	394	-	-	14/39/64/64	0/5/5/5
2	PB8	A	394	-	-	7/39/64/64	0/5/5/5

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	394	PB8	C7-C14	7.87	1.52	1.39
2	E	394	PB8	C27-C19	-6.01	1.47	1.52
2	B	394	PB8	C6-C13	5.77	1.49	1.39
2	D	394	PB8	C27-C19	-5.69	1.47	1.52
2	D	394	PB8	C14-C13	-5.69	1.29	1.40

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	394	PB8	C25-N40-C19	-9.94	107.14	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	394	PB8	O43-C19-C27	-9.87	118.06	126.75
2	B	394	PB8	C28-C20-N41	9.66	127.95	115.94
2	E	394	PB8	C16-C10-C17	8.70	126.33	118.75
2	E	394	PB8	O43-C19-C27	-8.47	119.30	126.75

There are no chirality outliers.

5 of 46 torsion outliers are listed below:

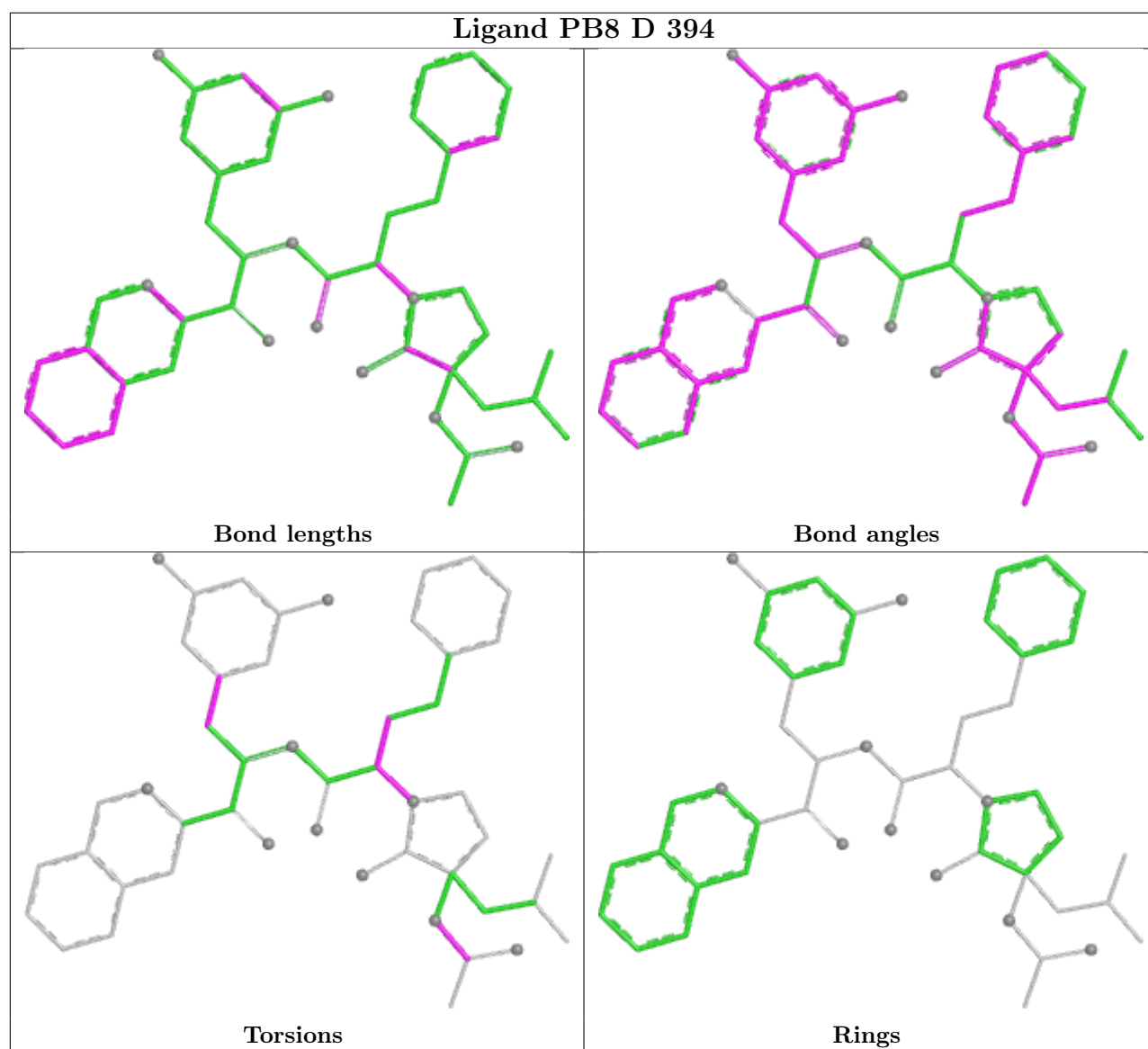
Mol	Chain	Res	Type	Atoms
2	A	394	PB8	C28-C20-N41-C27
2	A	394	PB8	O44-C20-N41-C27
2	A	394	PB8	N39-C26-C36-O46
2	B	394	PB8	C28-C20-N41-C27
2	B	394	PB8	O44-C20-N41-C27

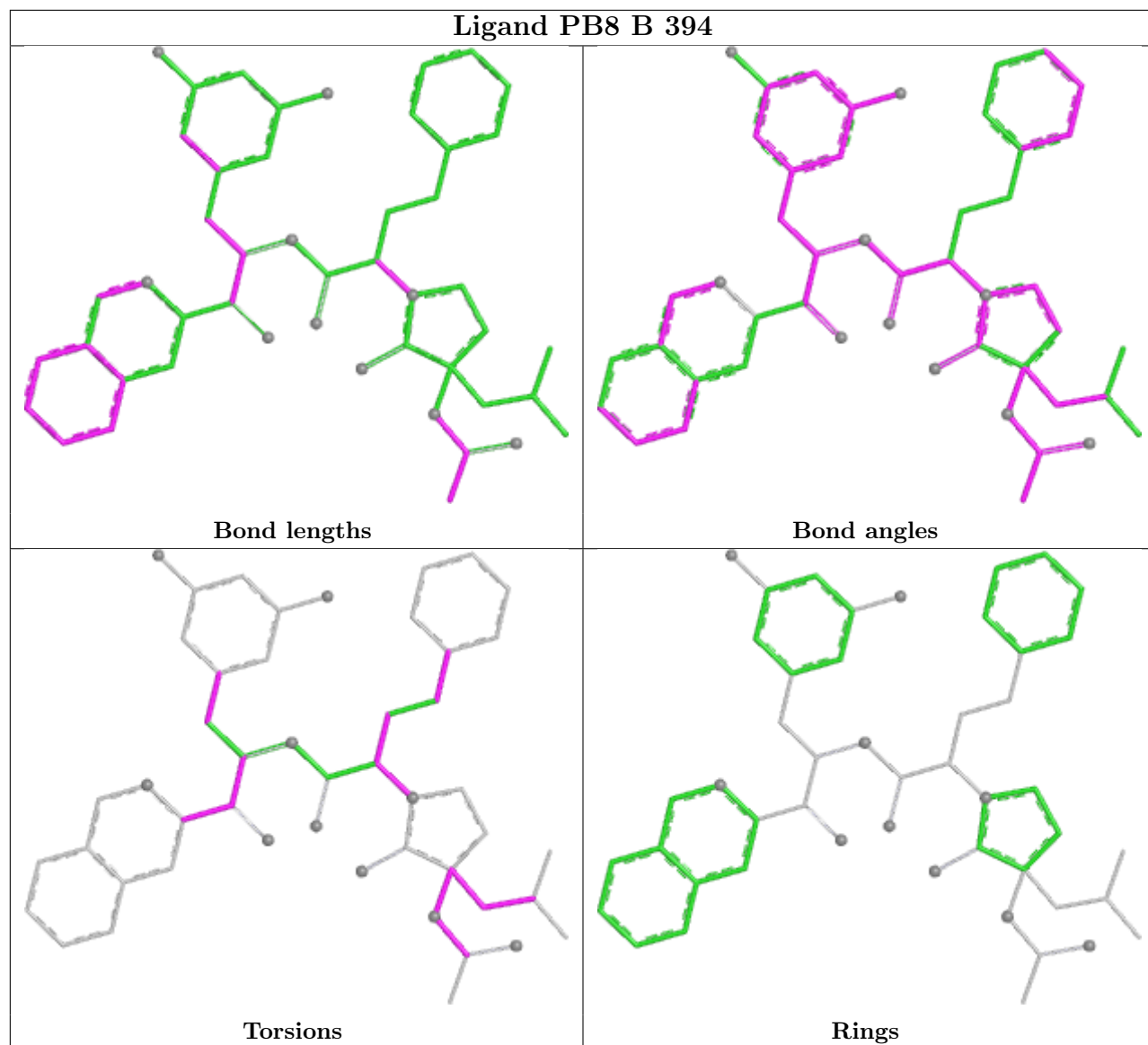
There are no ring outliers.

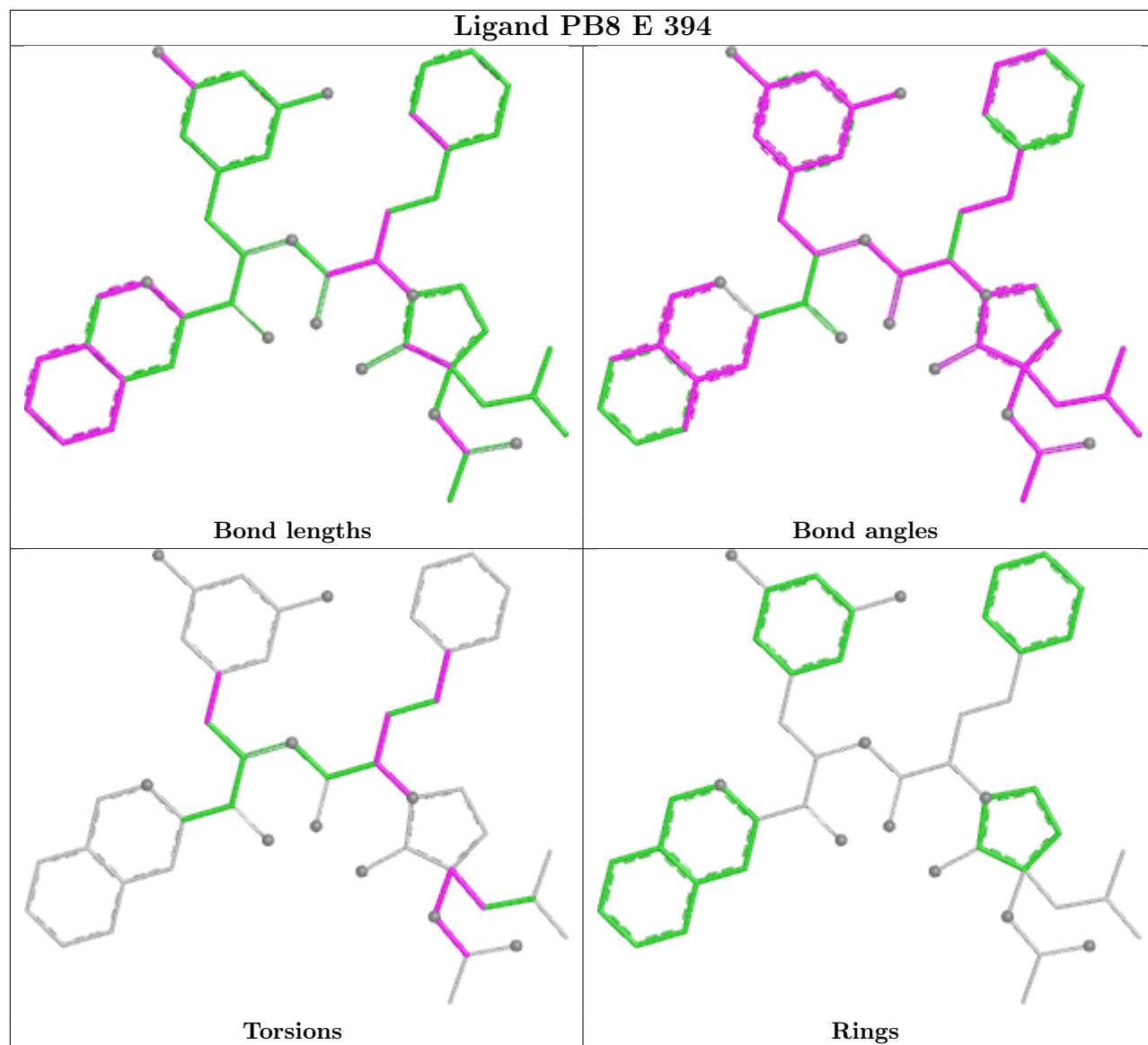
4 monomers are involved in 31 short contacts:

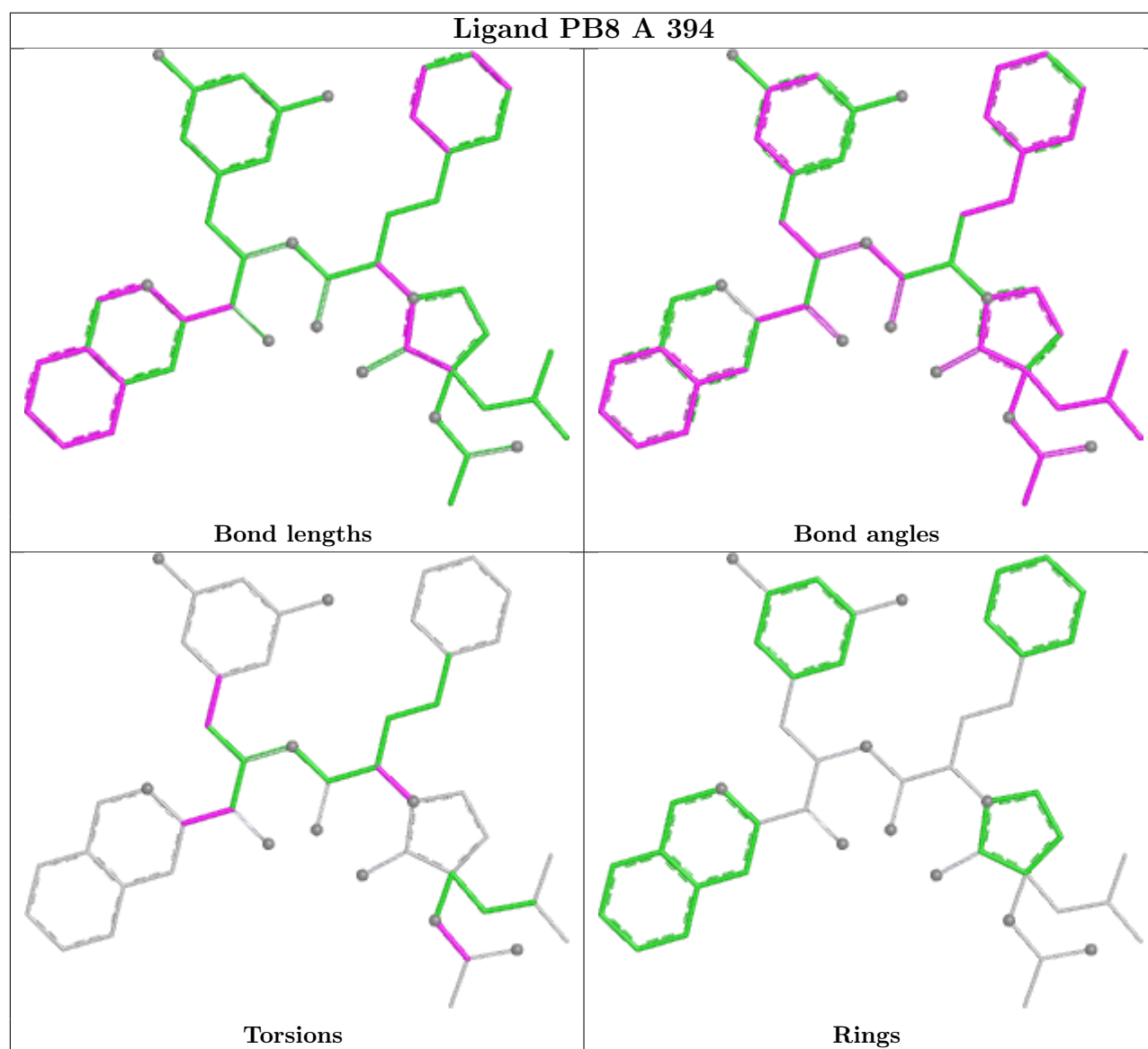
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	394	PB8	5	0
2	B	394	PB8	7	0
2	E	394	PB8	10	0
2	A	394	PB8	9	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	386/455 (84%)	0.23	13 (3%) 48 42	4, 18, 36, 59	0
1	B	386/455 (84%)	0.12	9 (2%) 61 55	3, 16, 35, 47	0
1	D	386/455 (84%)	0.50	19 (4%) 36 31	10, 24, 39, 59	0
1	E	386/455 (84%)	0.49	22 (5%) 30 26	10, 23, 41, 57	0
All	All	1544/1820 (84%)	0.33	63 (4%) 42 36	3, 20, 38, 59	0

The worst 5 of 63 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	376	THR	5.4
1	B	314	THR	5.4
1	E	312	VAL	4.8
1	D	377	LEU	4.7
1	B	376	THR	4.6

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](#)

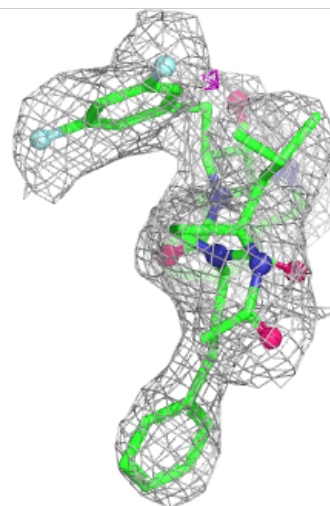
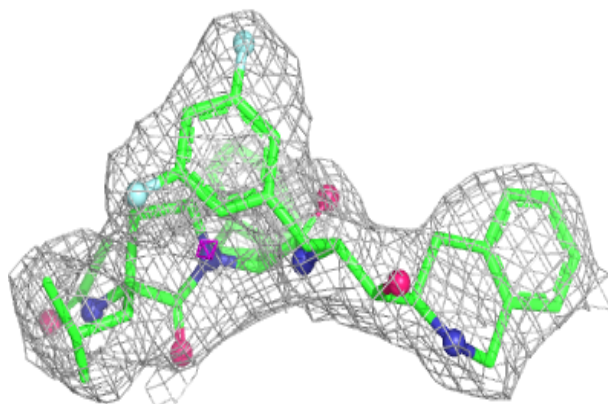
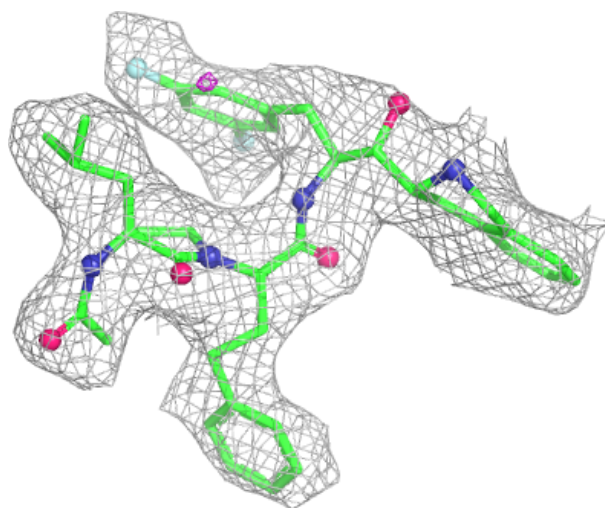
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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	PB8	E	394	48/48	0.91	0.12	6,15,20,22	0
2	PB8	A	394	48/48	0.92	0.11	2,11,21,24	0
2	PB8	D	394	48/48	0.93	0.11	3,15,24,25	0
2	PB8	B	394	48/48	0.93	0.10	3,10,15,20	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.

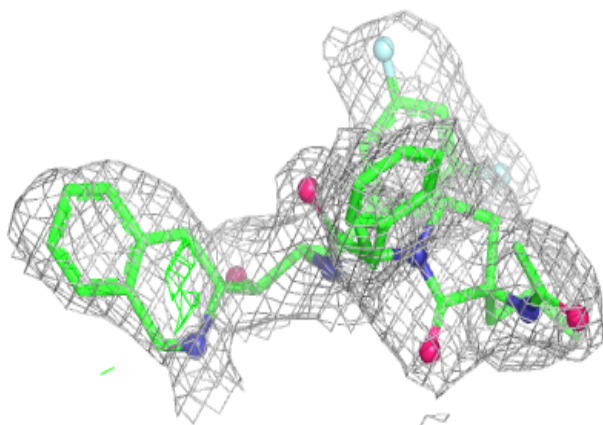
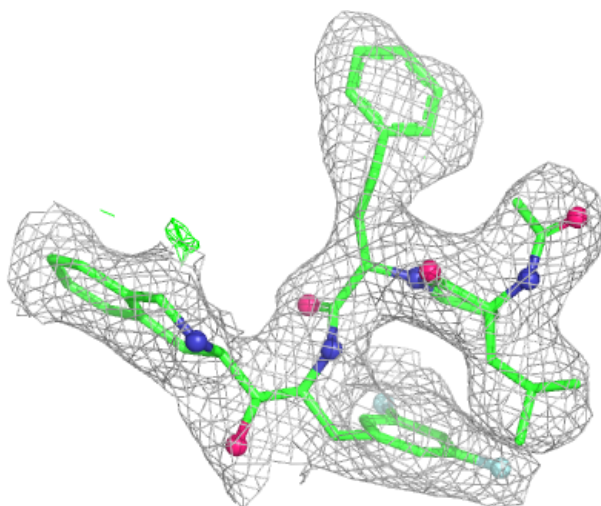
Electron density around PB8 E 394:

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



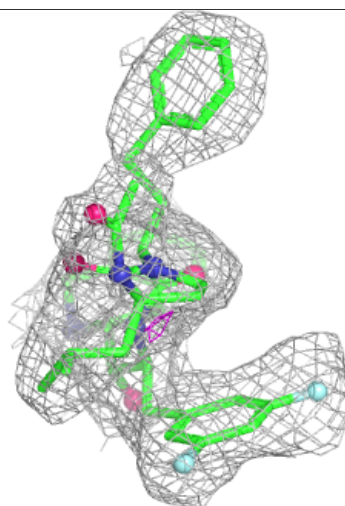
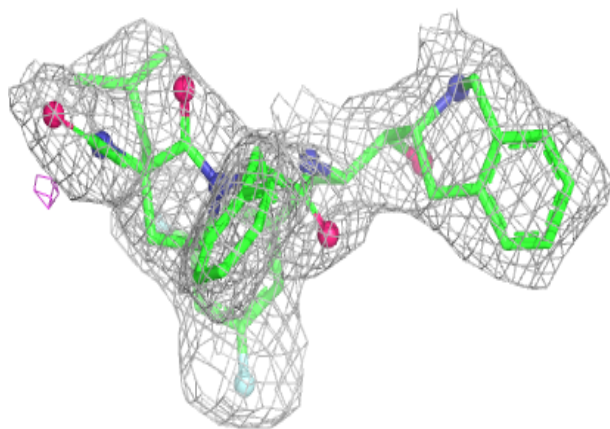
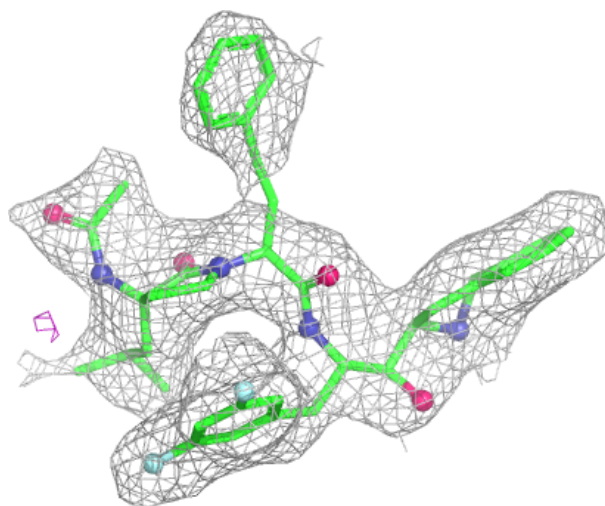
Electron density around PB8 A 394:

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



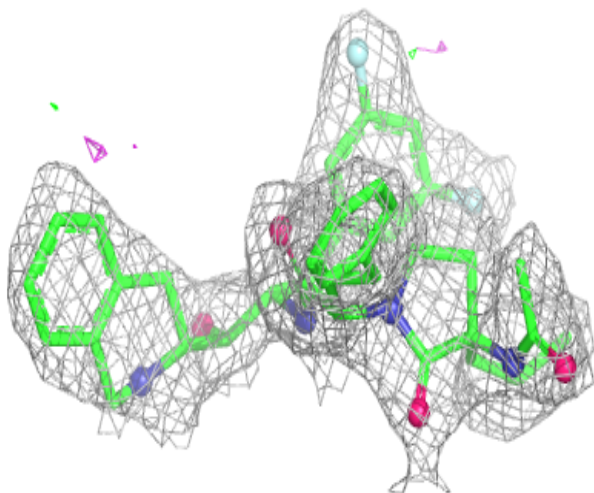
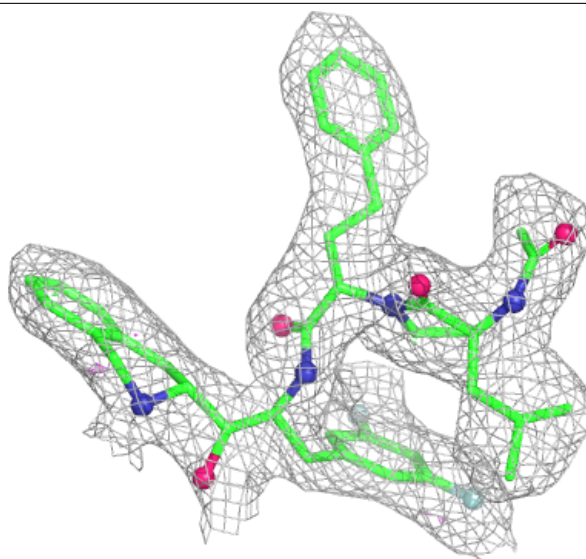
Electron density around PB8 D 394:

$2mF_o-DF_c$ (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-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.