



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:38 PM UTC

PDB ID : 8RDX / pdb_00008rdx
Title : PGGtase I in complex with probe BAY-6092
Authors : Steuber, H.
Deposited on : 2023-12-08
Resolution : 3.67 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

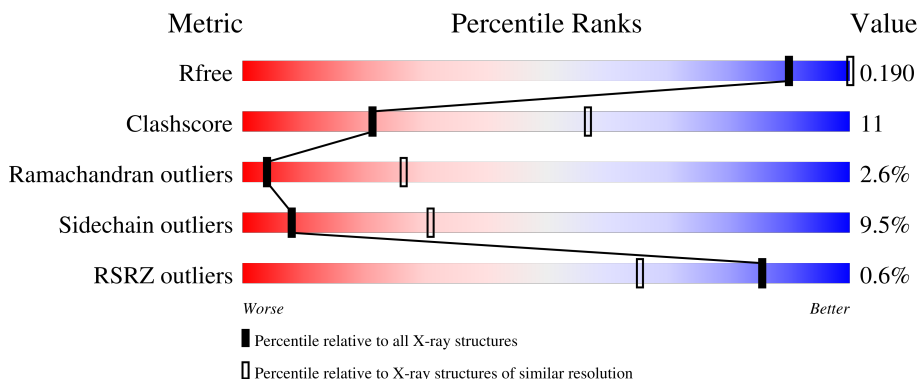
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.67 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1263 (3.80-3.56)
Clashscore	190562	1305 (3.80-3.56)
Ramachandran outliers	187476	1259 (3.80-3.56)
Sidechain outliers	187428	1256 (3.80-3.56)
RSRZ outliers	180081	1262 (3.80-3.56)

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	314	68% 29% . .
1	C	314	64% 32% .
1	E	314	% 68% 27% .
1	G	314	% 63% 32% .
1	I	314	70% 25% 5%

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Mol	Chain	Length	Quality of chain
1	K	314	 66% 29% 5%
2	B	346	 % 71% 23% 6%
2	D	346	 65% 29% 6%
2	F	346	 % 70% 26% ..
2	H	346	 66% 29% ..
2	J	346	 68% 27% .
2	L	346	 % 59% 34% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DPO	D	403	-	-	X	-
5	DPO	H	403	-	-	X	-
5	DPO	J	403	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 32241 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 Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	314	2629	1679	463	482	5	0	0	0
1	C	314	2629	1679	463	482	5	0	0	0
1	E	314	2632	1680	463	484	5	0	0	0
1	G	314	2629	1679	463	482	5	0	0	0
1	I	314	2629	1679	463	482	5	0	0	0
1	K	314	2629	1679	463	482	5	0	0	0

- Molecule 2 is a protein called Geranylgeranyl transferase type-1 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	346	2697	1707	467	499	24	0	0	0
2	D	346	2697	1707	467	499	24	0	0	0
2	F	346	2697	1707	467	499	24	0	0	0
2	H	346	2697	1707	467	499	24	0	0	0
2	J	346	2697	1707	467	499	24	0	0	0
2	L	346	2697	1707	467	499	24	0	0	0

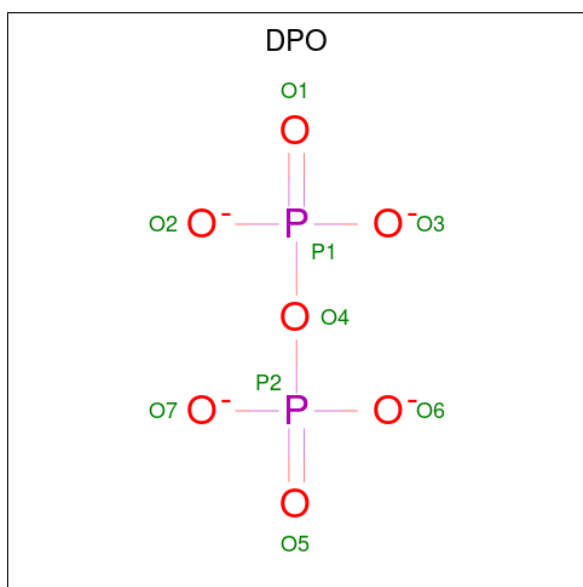
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	D	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0
3	J	1	Total 1	Zn 1	0	0
3	L	1	Total 1	Zn 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

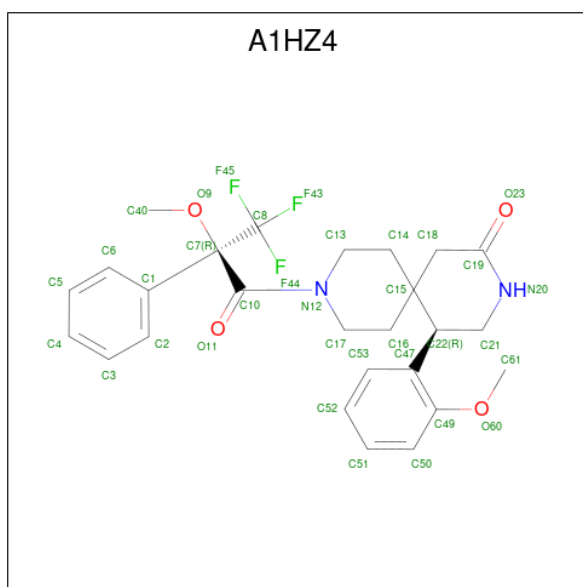
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	F	1	Total 1	Cl 1	0	0
4	H	1	Total 1	Cl 1	0	0
4	J	1	Total 1	Cl 1	0	0
4	L	1	Total 1	Cl 1	0	0

- Molecule 5 is DIPHOSPHATE (CCD ID: DPO) (formula: O₇P₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total O P 9 7 2	0	0
5	D	1	Total O P 9 7 2	0	0
5	F	1	Total O P 9 7 2	0	0
5	H	1	Total O P 9 7 2	0	0
5	J	1	Total O P 9 7 2	0	0
5	L	1	Total O P 9 7 2	0	0

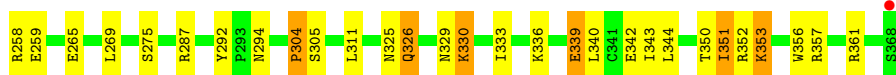
- Molecule 6 is (5 {R})-5-(2-methoxyphenyl)-9-[(2 {R})-3,3,3-tris(fluoranyl)-2-methoxy-2-phenyl-propanoyl]-3,9-diazaspiro[5.5]undecan-2-one (CCD ID: A1HZ4) (formula: C₂₆H₂₉F₃N₂O₄) (labeled as "Ligand of Interest" by depositor).



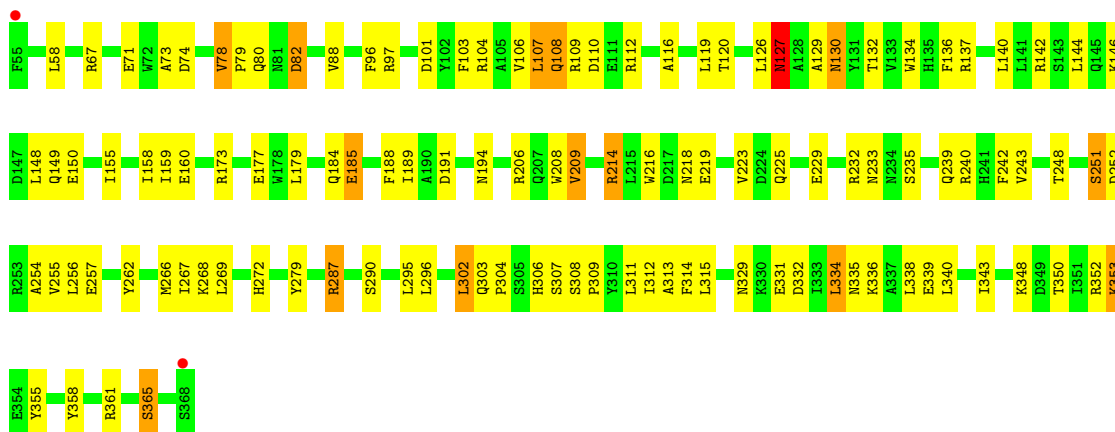
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
6	B	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	D	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	F	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	H	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	J	1	Total 35	C 26	F 3	N 2	O 4	0	0
6	L	1	Total 35	C 26	F 3	N 2	O 4	0	0

- Molecule 7 is water.

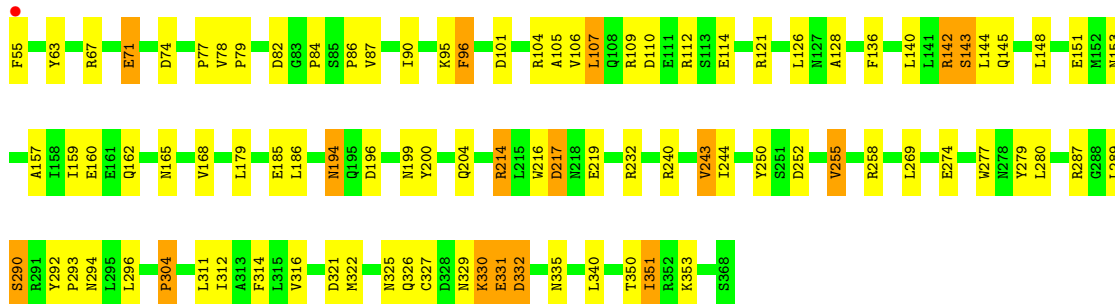
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	O 1	0	0
7	D	1	Total 1	O 1	0	0
7	F	1	Total 1	O 1	0	0
7	H	1	Total 1	O 1	0	0
7	J	1	Total 1	O 1	0	0
7	L	1	Total 1	O 1	0	0



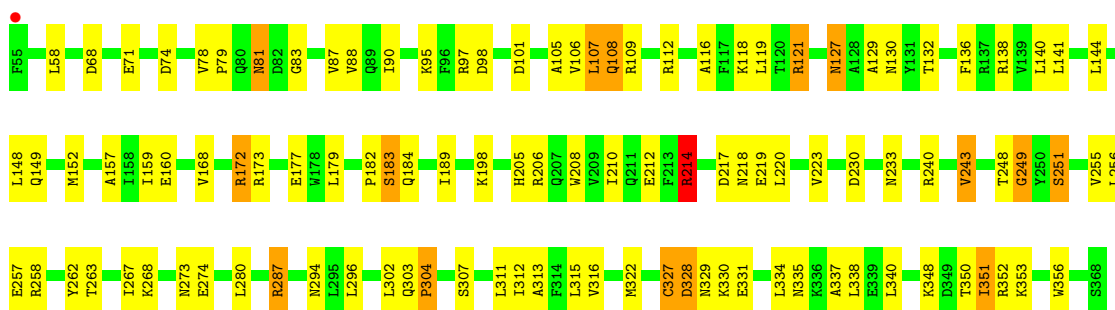
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



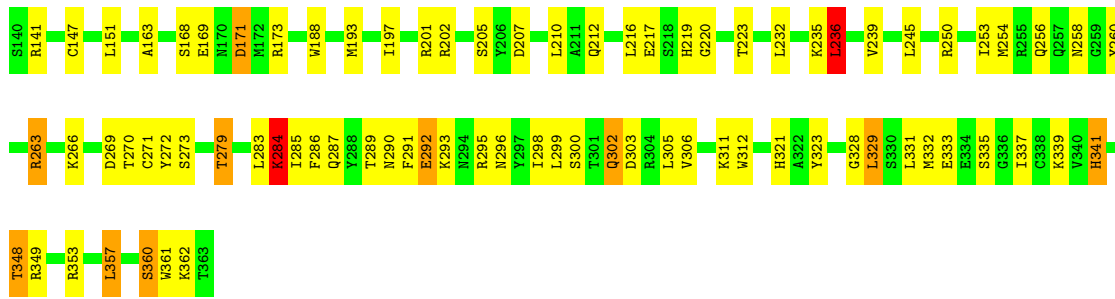
- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha



- Molecule 1: Protein farnesyltransferase/geranylgeranyltransferase type-1 subunit alpha

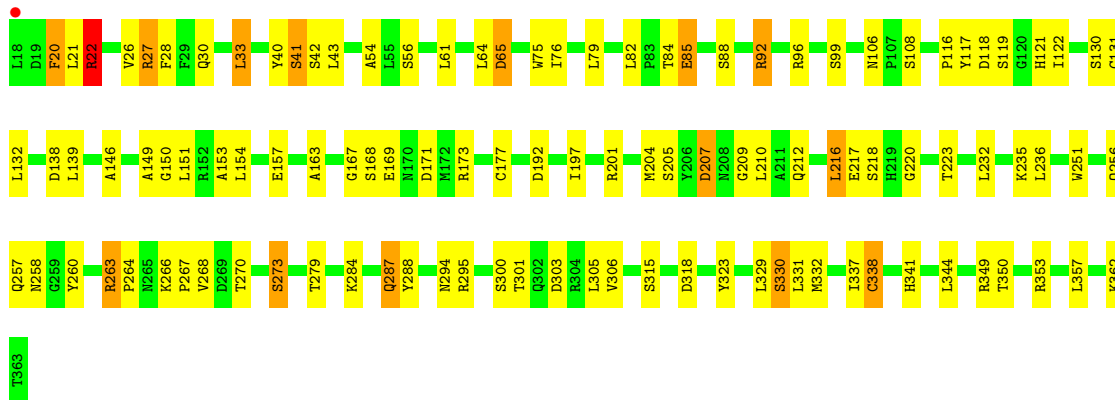


- Molecule 2: Geranylgeranyl transferase type-1 subunit beta



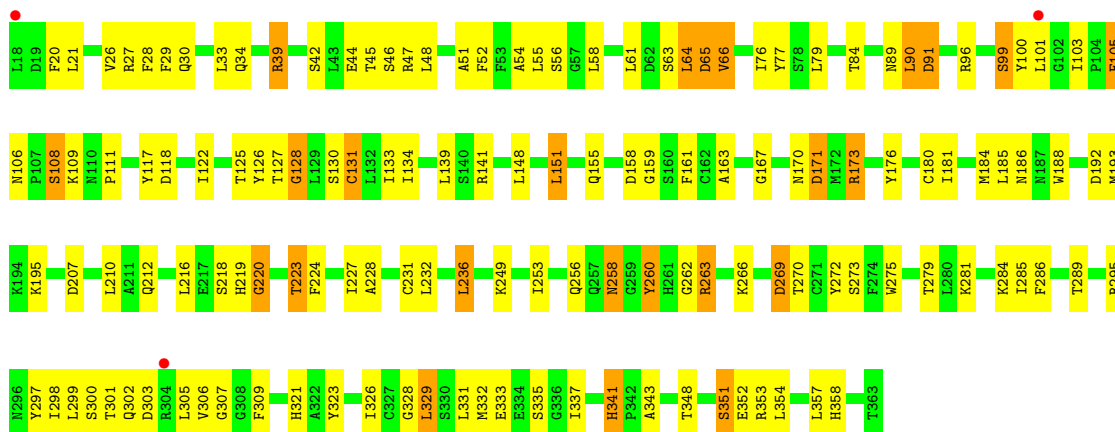
- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain J: 68% 27%



- Molecule 2: Geranylgeranyl transferase type-1 subunit beta

Chain L: 59% 34% 7%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	270.89Å 269.26Å 185.25Å 90.00° 131.77° 90.00°	Depositor
Resolution (Å)	48.21 – 3.67 48.21 – 3.67	Depositor EDS
% Data completeness (in resolution range)	97.9 (48.21-3.67) 97.9 (48.21-3.67)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 3.67Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.137 , 0.189 0.147 , 0.190	Depositor DCC
R_{free} test set	2100 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	94.8	Xtrriage
Anisotropy	0.487	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.087 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	32241	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DPO, A1HZ4, ZN, CL

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	1.03	0/2695	1.59	16/3668 (0.4%)
1	C	1.03	0/2695	1.59	13/3668 (0.4%)
1	E	1.04	0/2698	1.60	7/3672 (0.2%)
1	G	1.04	0/2695	1.57	9/3668 (0.2%)
1	I	1.04	0/2695	1.58	10/3668 (0.3%)
1	K	1.03	0/2695	1.57	9/3668 (0.2%)
2	B	1.07	0/2759	1.63	20/3733 (0.5%)
2	D	1.09	2/2759 (0.1%)	1.60	14/3733 (0.4%)
2	F	1.09	0/2759	1.60	19/3733 (0.5%)
2	H	1.07	2/2759 (0.1%)	1.63	13/3733 (0.3%)
2	J	1.08	1/2759 (0.0%)	1.63	20/3733 (0.5%)
2	L	1.10	0/2759	1.60	15/3733 (0.4%)
All	All	1.06	5/32727 (0.0%)	1.60	165/44410 (0.4%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	273	SER	C-O	6.18	1.31	1.24
2	D	81	VAL	C-O	5.51	1.29	1.24
2	H	81	VAL	C-O	5.41	1.29	1.24
2	H	273	SER	C-O	5.20	1.30	1.24
2	J	273	SER	C-O	5.12	1.30	1.24

The worst 5 of 165 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	258	ASN	N-CA-C	-9.78	99.92	112.93
2	B	65	ASP	CA-CB-CG	8.16	120.76	112.60
2	J	258	ASN	N-CA-C	-7.98	102.07	112.68
1	K	68	ASP	CA-CB-CG	7.33	119.93	112.60
2	J	167	GLY	CA-C-O	-7.19	117.55	122.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2629	0	2520	59	0
1	C	2629	0	2520	62	0
1	E	2632	0	2522	58	0
1	G	2629	0	2520	67	0
1	I	2629	0	2520	49	0
1	K	2629	0	2520	64	0
2	B	2697	0	2600	52	0
2	D	2697	0	2600	70	0
2	F	2697	0	2600	51	0
2	H	2697	0	2600	56	0
2	J	2697	0	2600	57	0
2	L	2697	0	2600	80	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	J	1	0	0	0	0
3	L	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
4	J	1	0	0	0	0
4	L	1	0	0	0	0
5	B	9	0	0	0	0
5	D	9	0	0	2	0
5	F	9	0	0	0	0
5	H	9	0	0	2	0
5	J	9	0	0	2	0
5	L	9	0	0	1	0
6	B	35	0	0	0	0
6	D	35	0	0	0	0
6	F	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	35	0	0	1	0
6	J	35	0	0	0	0
6	L	35	0	0	0	0
7	B	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	H	1	0	0	0	0
7	J	1	0	0	0	0
7	L	1	0	0	0	0
All	All	32241	0	30722	688	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 11.

The worst 5 of 688 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)
6:H:404:A1HZ4:C40	6:H:404:A1HZ4:C2	2.31	1.08
2:F:258:ASN:OD1	2:F:268:VAL:HG21	1.72	0.90
2:B:259:GLY:O	2:B:268:VAL:CG1	2.21	0.89
1:I:296:LEU:HD22	1:I:322:MET:HE1	1.56	0.87
2:B:259:GLY:O	2:B:268:VAL:HG12	1.75	0.86

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	312/314 (99%)	266 (85%)	40 (13%)	6 (2%)	6 32
1	C	312/314 (99%)	257 (82%)	47 (15%)	8 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	312/314 (99%)	266 (85%)	37 (12%)	9 (3%)	3	25
1	G	312/314 (99%)	255 (82%)	52 (17%)	5 (2%)	7	34
1	I	312/314 (99%)	254 (81%)	42 (14%)	16 (5%)	1	16
1	K	312/314 (99%)	255 (82%)	48 (15%)	9 (3%)	3	25
2	B	344/346 (99%)	297 (86%)	39 (11%)	8 (2%)	5	29
2	D	344/346 (99%)	301 (88%)	34 (10%)	9 (3%)	4	26
2	F	344/346 (99%)	301 (88%)	38 (11%)	5 (2%)	8	35
2	H	344/346 (99%)	296 (86%)	37 (11%)	11 (3%)	3	24
2	J	344/346 (99%)	299 (87%)	40 (12%)	5 (2%)	8	35
2	L	344/346 (99%)	281 (82%)	50 (14%)	13 (4%)	2	20
All	All	3936/3960 (99%)	3328 (85%)	504 (13%)	104 (3%)	4	26

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	110	ASP
1	A	326	GLN
1	A	329	ASN
2	B	137	ASP
1	C	304	PRO

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	280/293 (96%)	258 (92%)	22 (8%)	11	37
1	C	280/293 (96%)	257 (92%)	23 (8%)	10	35
1	E	281/293 (96%)	254 (90%)	27 (10%)	8	30
1	G	280/293 (96%)	254 (91%)	26 (9%)	8	31
1	I	280/293 (96%)	260 (93%)	20 (7%)	13	40
1	K	280/293 (96%)	257 (92%)	23 (8%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	289/301 (96%)	257 (89%)	32 (11%)	6	25
2	D	289/301 (96%)	256 (89%)	33 (11%)	5	24
2	F	289/301 (96%)	259 (90%)	30 (10%)	7	28
2	H	289/301 (96%)	257 (89%)	32 (11%)	6	25
2	J	289/301 (96%)	263 (91%)	26 (9%)	9	32
2	L	289/301 (96%)	258 (89%)	31 (11%)	6	27
All	All	3415/3564 (96%)	3090 (90%)	325 (10%)	8	31

5 of 325 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	109	ARG
1	K	287	ARG
1	I	232	ARG
2	J	300	SER
2	L	99	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	238	ASN
1	K	218	ASN
1	I	306	HIS
2	J	265	ASN
1	K	367	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](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 12 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	A1HZ4	L	404	-	38,38,38	1.95	8 (21%)	49,57,57	2.72	20 (40%)
6	A1HZ4	B	404	-	38,38,38	1.81	8 (21%)	49,57,57	2.30	14 (28%)
6	A1HZ4	D	404	-	38,38,38	1.94	5 (13%)	49,57,57	2.55	16 (32%)
5	DPO	B	403	-	6,8,8	0.65	0	12,13,13	0.94	0
5	DPO	L	403	-	6,8,8	0.92	0	12,13,13	0.73	0
6	A1HZ4	F	404	-	38,38,38	1.86	9 (23%)	49,57,57	2.43	18 (36%)
6	A1HZ4	J	404	-	38,38,38	1.88	5 (13%)	49,57,57	2.50	18 (36%)
6	A1HZ4	H	404	-	38,38,38	2.00	5 (13%)	49,57,57	2.54	17 (34%)
5	DPO	F	403	-	6,8,8	1.07	1 (16%)	12,13,13	0.80	0
5	DPO	H	403	-	6,8,8	0.60	0	12,13,13	0.87	0
5	DPO	J	403	-	6,8,8	0.70	0	12,13,13	0.82	0
5	DPO	D	403	-	6,8,8	0.94	0	12,13,13	0.74	0

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
6	A1HZ4	L	404	-	-	0/34/62/62	0/4/4/4
6	A1HZ4	B	404	-	-	0/34/62/62	0/4/4/4
6	A1HZ4	D	404	-	-	5/34/62/62	0/4/4/4
5	DPO	B	403	-	-	2/6/6/6	-
5	DPO	L	403	-	-	0/6/6/6	-
6	A1HZ4	F	404	-	-	8/34/62/62	0/4/4/4
6	A1HZ4	J	404	-	-	1/34/62/62	0/4/4/4
6	A1HZ4	H	404	-	-	0/34/62/62	0/4/4/4
5	DPO	F	403	-	-	4/6/6/6	-
5	DPO	H	403	-	-	0/6/6/6	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DPO	J	403	-	-	4/6/6/6	-
5	DPO	D	403	-	-	4/6/6/6	-

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	404	A1HZ4	C21-N20	6.80	1.53	1.46
6	B	404	A1HZ4	C21-N20	6.48	1.52	1.46
6	L	404	A1HZ4	C21-N20	6.24	1.52	1.46
6	F	404	A1HZ4	O9-C7	6.12	1.53	1.41
6	H	404	A1HZ4	C21-N20	6.10	1.52	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	404	A1HZ4	C7-C10-N12	10.44	128.20	117.64
6	H	404	A1HZ4	C7-C10-N12	9.79	127.54	117.64
6	J	404	A1HZ4	C7-C10-N12	9.38	127.13	117.64
6	B	404	A1HZ4	O60-C49-C47	8.01	123.79	115.84
6	D	404	A1HZ4	C7-C10-N12	7.66	125.39	117.64

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

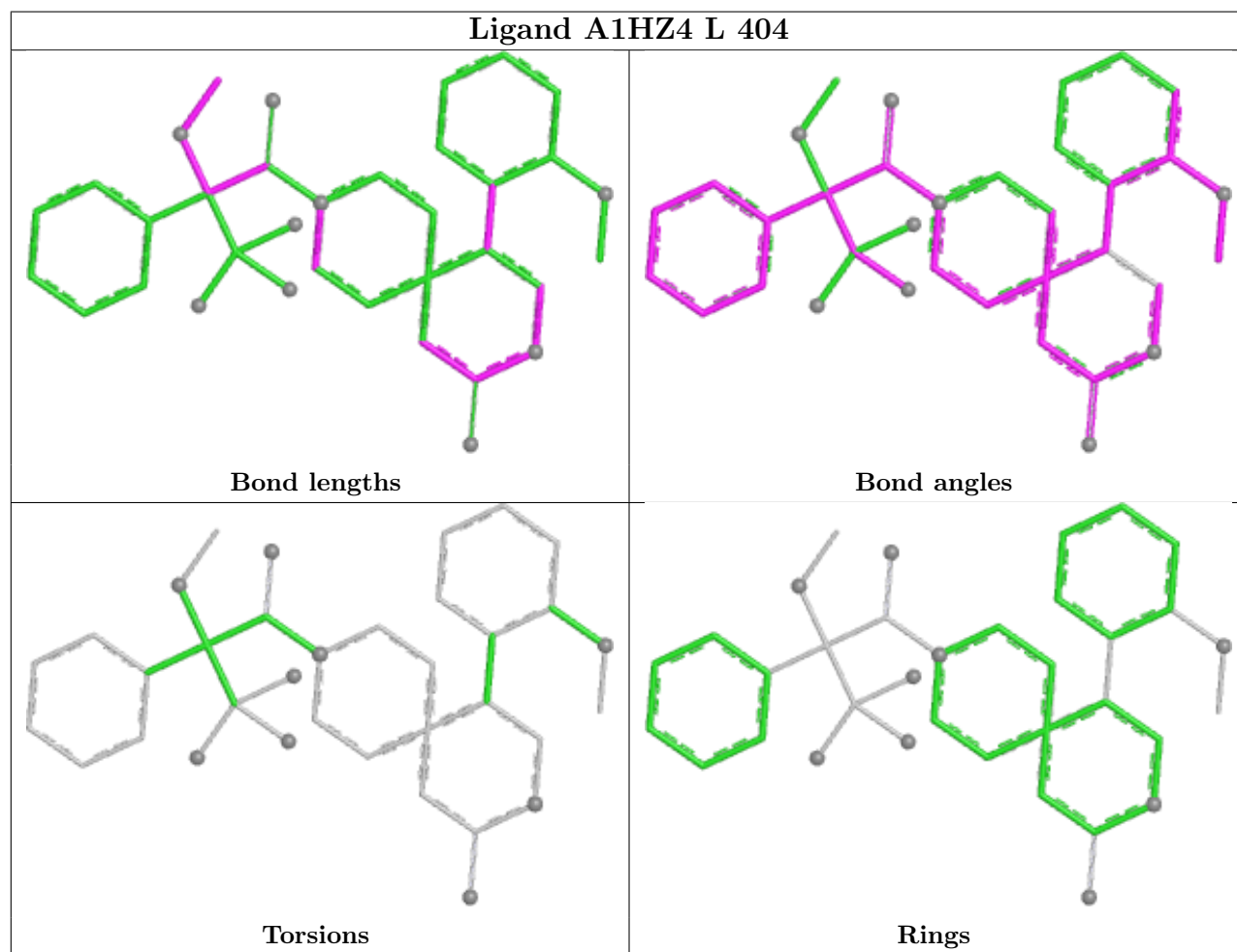
Mol	Chain	Res	Type	Atoms
5	D	403	DPO	P1-O4-P2-O7
5	J	403	DPO	P2-O4-P1-O2
5	J	403	DPO	P1-O4-P2-O7
6	D	404	A1HZ4	C8-C7-O9-C40
6	F	404	A1HZ4	C10-C7-C8-F44

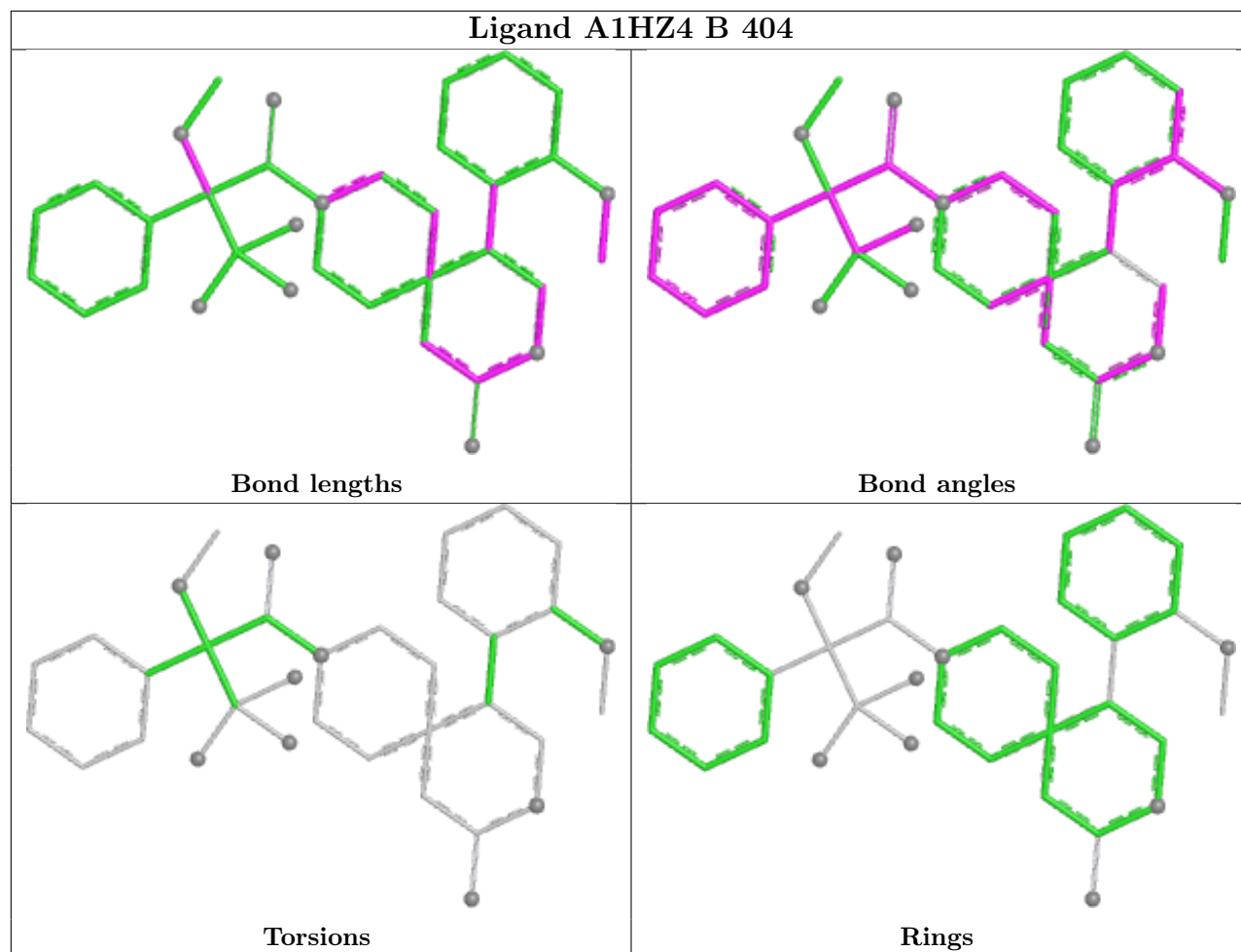
There are no ring outliers.

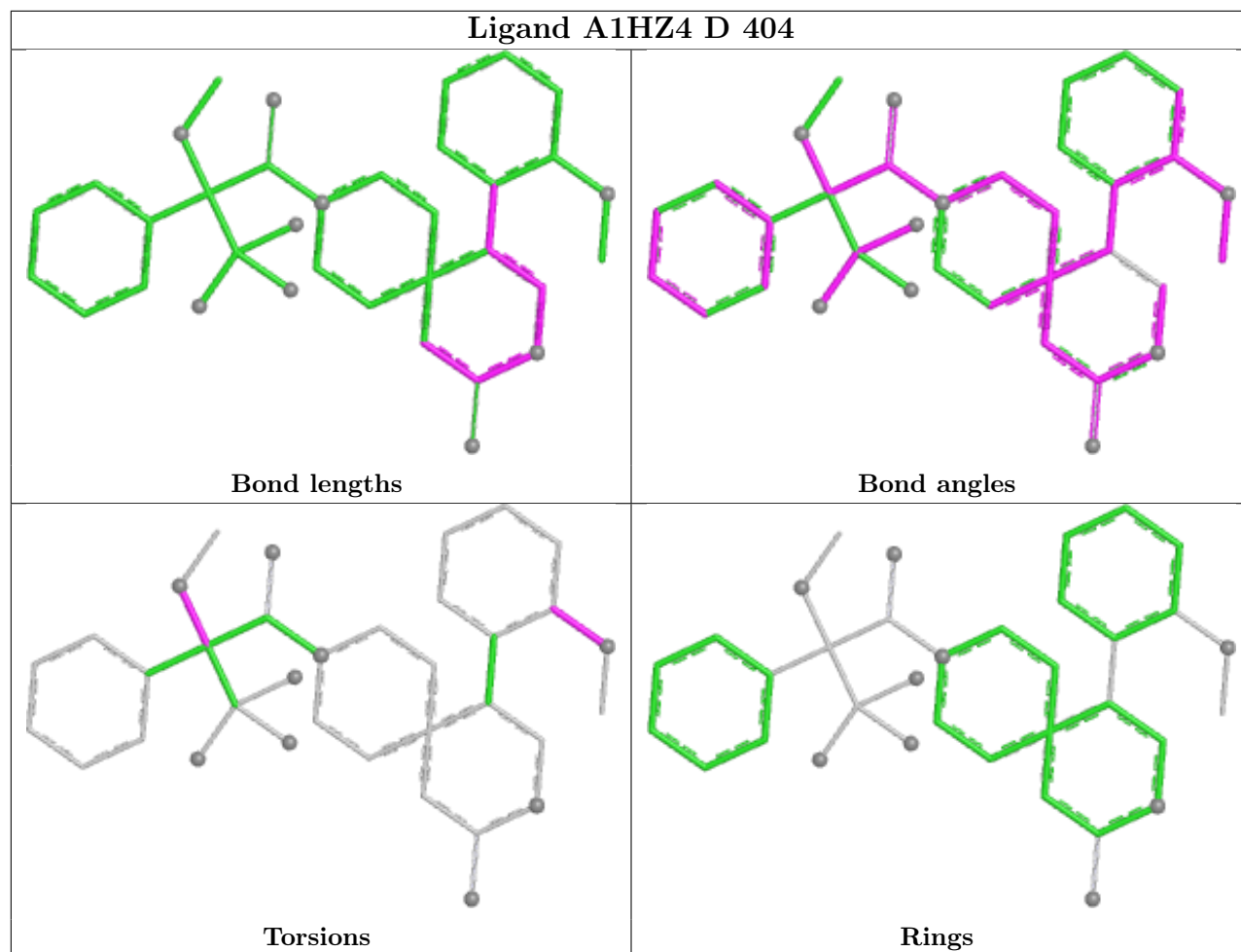
5 monomers are involved in 8 short contacts:

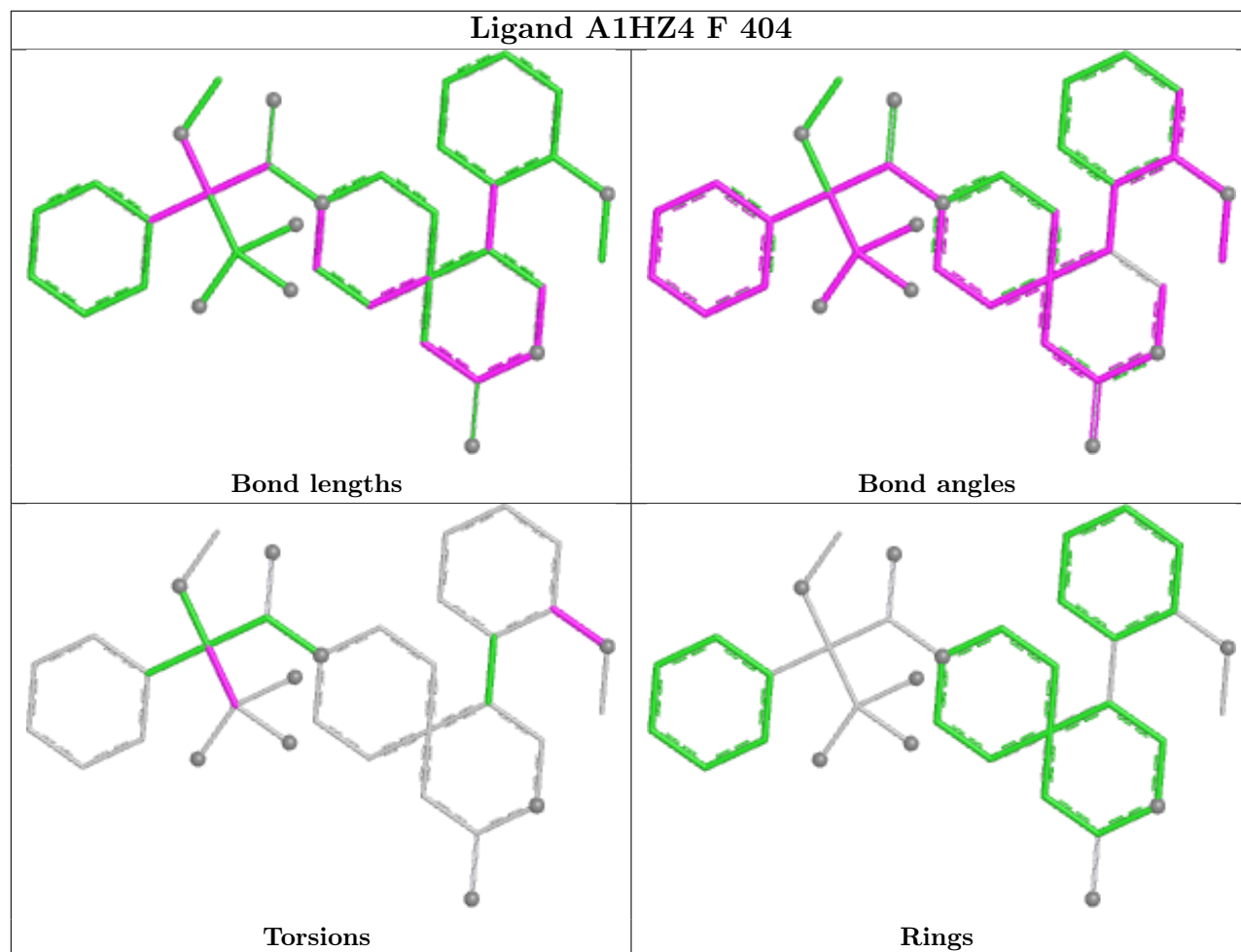
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	403	DPO	1	0
6	H	404	A1HZ4	1	0
5	H	403	DPO	2	0
5	J	403	DPO	2	0
5	D	403	DPO	2	0

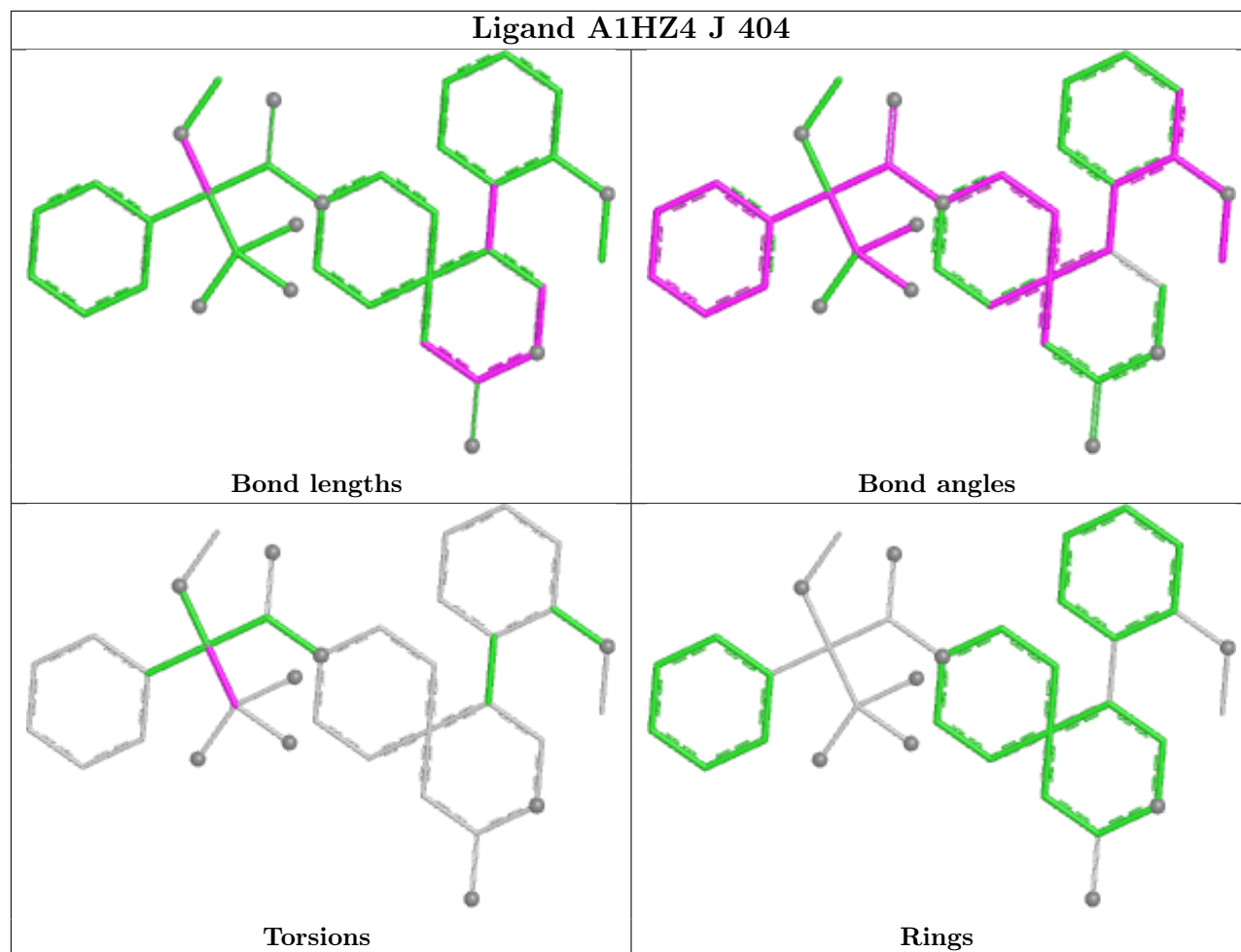
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

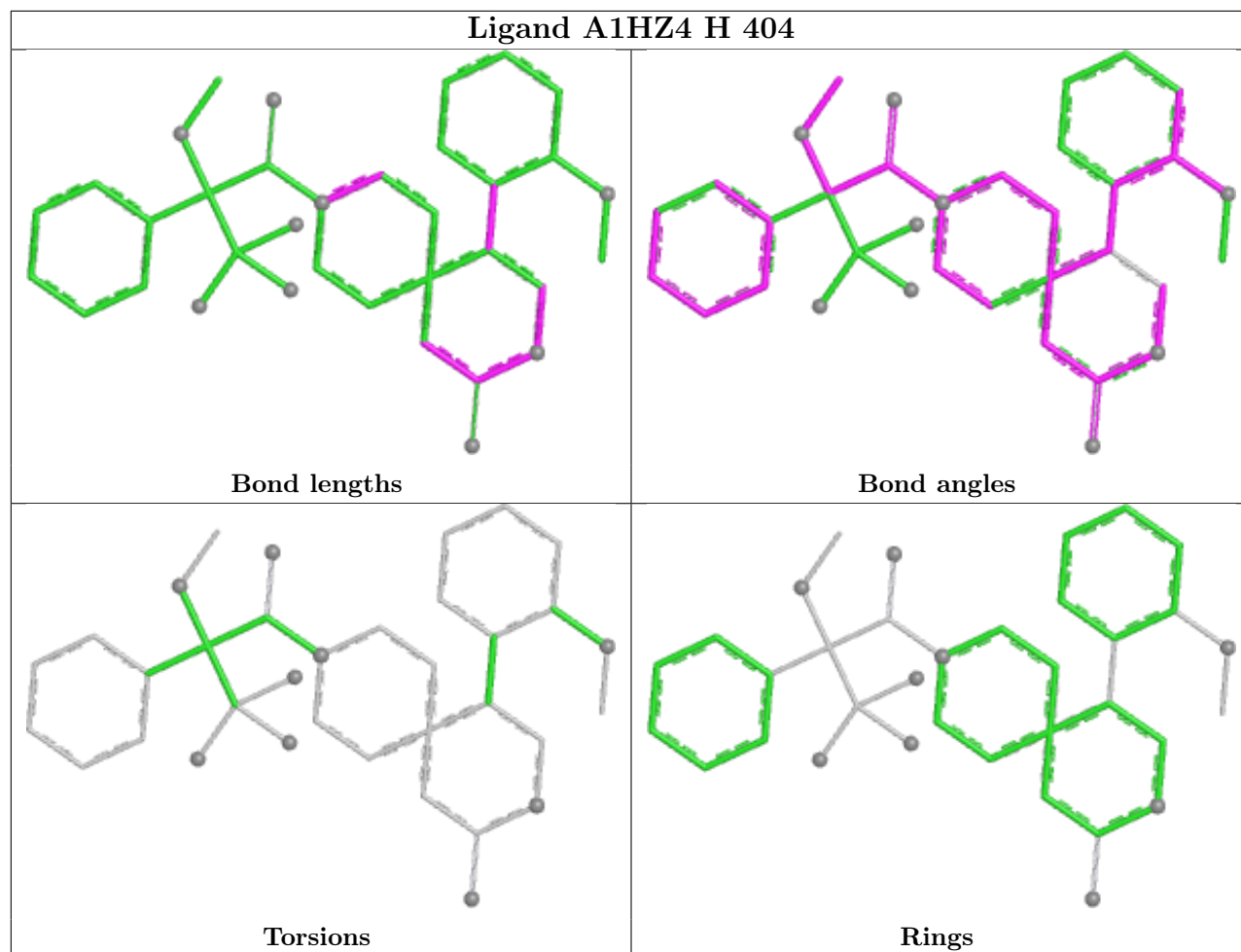












5.7 Other polymers [i](#)

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	314/314 (100%)	-0.71	1 (0%) 90 76	52, 78, 111, 143	0
1	C	314/314 (100%)	-0.63	1 (0%) 90 76	58, 87, 122, 144	0
1	E	314/314 (100%)	-0.67	2 (0%) 85 65	56, 84, 123, 151	0
1	G	314/314 (100%)	-0.66	2 (0%) 85 65	60, 88, 125, 155	0
1	I	314/314 (100%)	-0.62	1 (0%) 90 76	62, 93, 135, 162	0
1	K	314/314 (100%)	-0.61	1 (0%) 90 76	62, 93, 131, 158	0
2	B	346/346 (100%)	-0.68	3 (0%) 81 57	50, 72, 108, 140	0
2	D	346/346 (100%)	-0.72	1 (0%) 90 76	50, 73, 109, 153	0
2	F	346/346 (100%)	-0.59	5 (1%) 73 47	58, 84, 126, 177	0
2	H	346/346 (100%)	-0.67	1 (0%) 90 76	57, 82, 120, 152	0
2	J	346/346 (100%)	-0.63	1 (0%) 90 76	62, 85, 119, 153	0
2	L	346/346 (100%)	-0.49	3 (0%) 81 57	62, 97, 140, 171	0
All	All	3960/3960 (100%)	-0.64	22 (0%) 85 65	50, 84, 126, 177	0

The worst 5 of 22 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	258	ASN	3.9
2	H	18	LEU	3.8
2	L	18	LEU	3.8
1	K	55	PHE	3.1
1	C	55	PHE	3.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

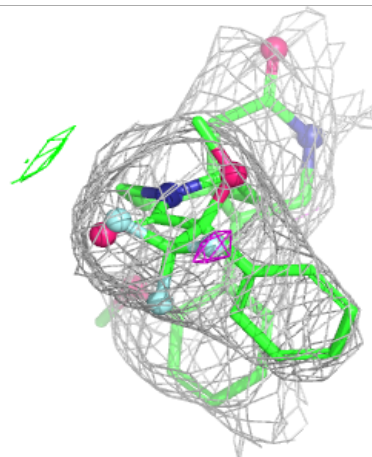
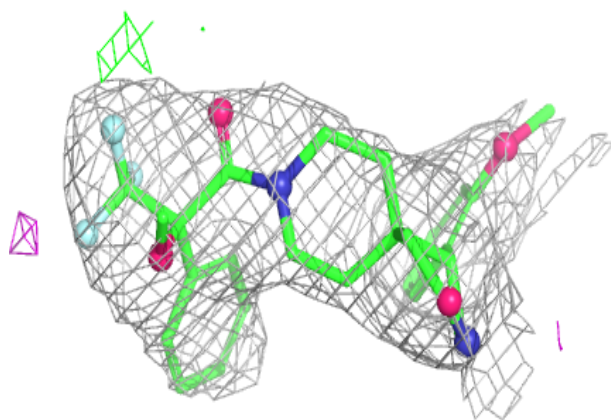
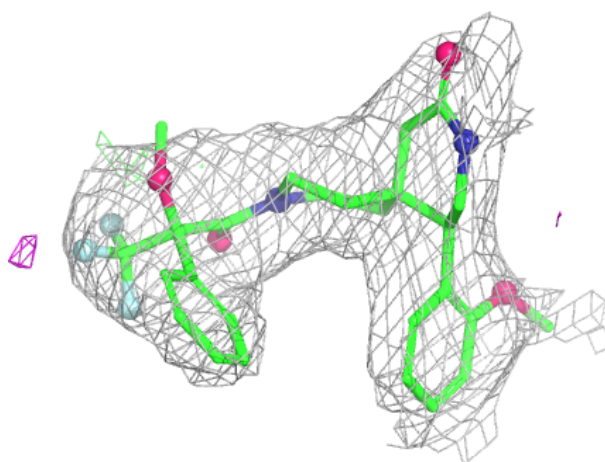
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DPO	J	403	9/9	0.87	0.09	117,130,149,151	0
5	DPO	H	403	9/9	0.89	0.08	116,124,150,182	0
4	CL	B	402	1/1	0.89	0.13	81,81,81,81	0
4	CL	L	402	1/1	0.90	0.15	76,76,76,76	0
5	DPO	D	403	9/9	0.90	0.09	114,129,145,161	0
4	CL	J	402	1/1	0.91	0.19	91,91,91,91	0
4	CL	D	402	1/1	0.91	0.19	70,70,70,70	0
5	DPO	B	403	9/9	0.91	0.10	118,130,152,169	0
4	CL	H	402	1/1	0.94	0.10	76,76,76,76	0
5	DPO	L	403	9/9	0.94	0.16	112,126,140,142	0
5	DPO	F	403	9/9	0.95	0.16	98,124,148,161	0
4	CL	F	402	1/1	0.95	0.12	88,88,88,88	0
6	A1HZ4	B	404	35/35	0.98	0.08	58,75,101,113	0
6	A1HZ4	D	404	35/35	0.98	0.08	61,78,93,109	0
6	A1HZ4	F	404	35/35	0.98	0.08	67,79,97,103	0
6	A1HZ4	H	404	35/35	0.98	0.08	74,82,111,120	0
6	A1HZ4	J	404	35/35	0.98	0.08	71,82,103,109	0
6	A1HZ4	L	404	35/35	0.98	0.09	73,92,116,125	0
3	ZN	L	401	1/1	0.99	0.04	70,70,70,70	0
3	ZN	J	401	1/1	1.00	0.02	64,64,64,64	0
3	ZN	B	401	1/1	1.00	0.02	50,50,50,50	0
3	ZN	D	401	1/1	1.00	0.01	63,63,63,63	0
3	ZN	F	401	1/1	1.00	0.02	61,61,61,61	0
3	ZN	H	401	1/1	1.00	0.01	63,63,63,63	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.

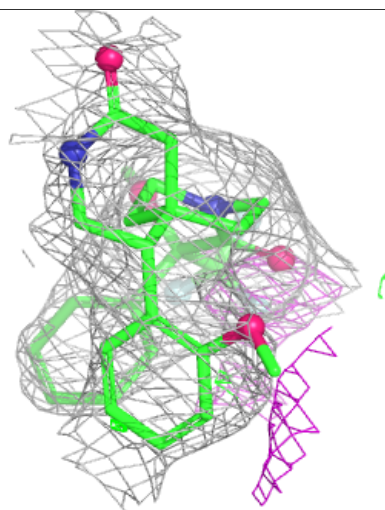
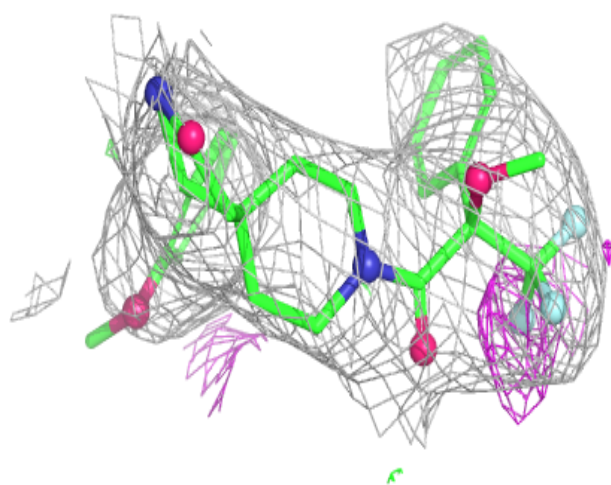
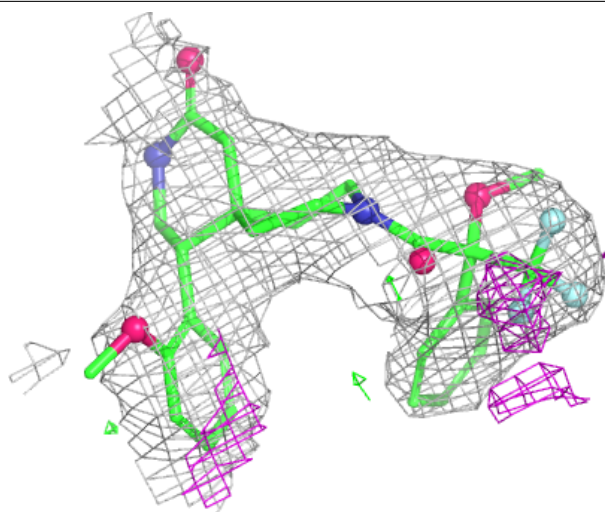
Electron density around A1HZ4 B 404:

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



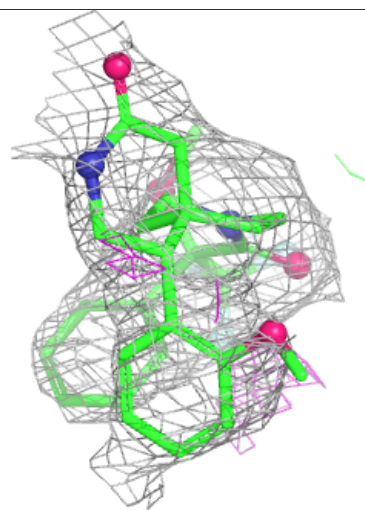
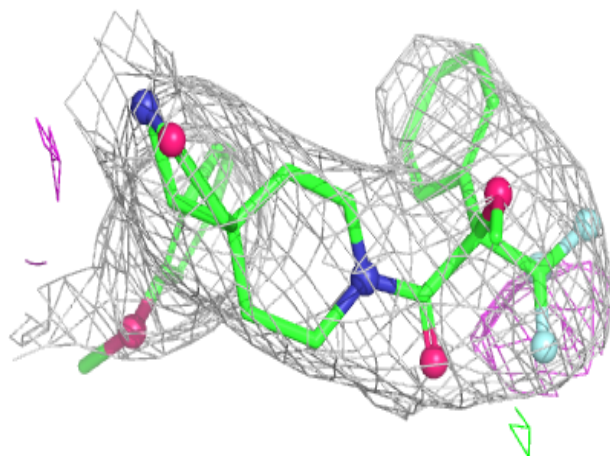
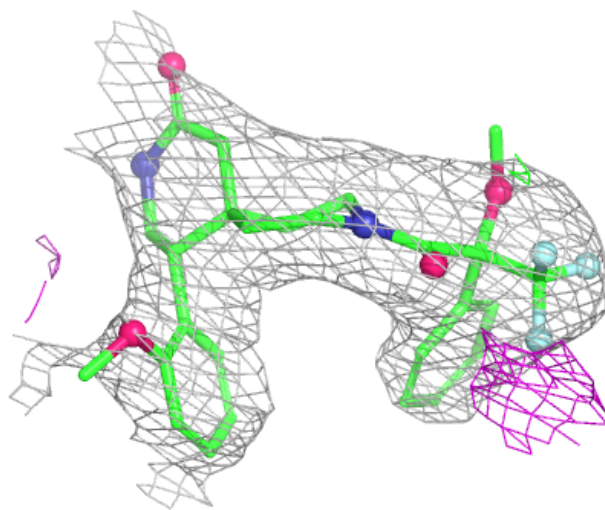
Electron density around A1HZ4 D 404:

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



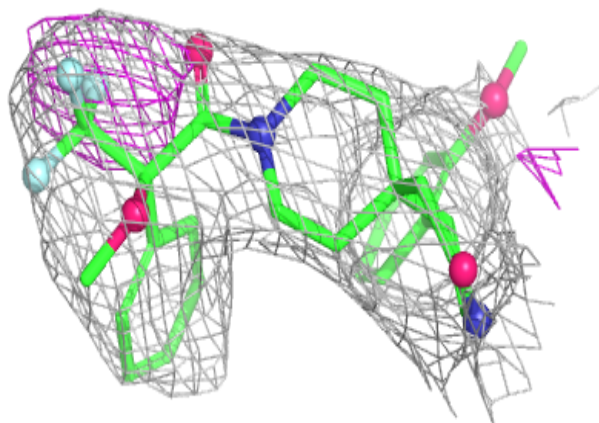
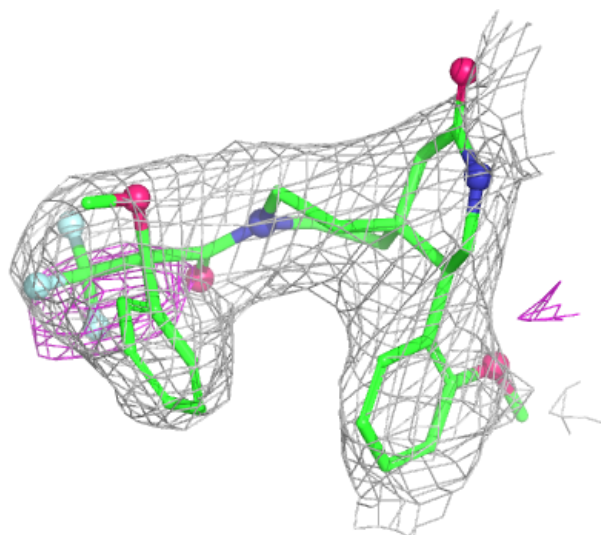
Electron density around A1HZ4 F 404:

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



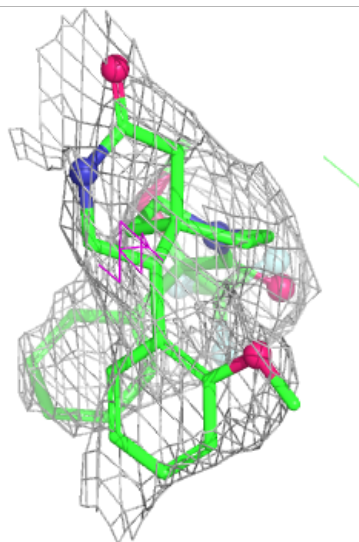
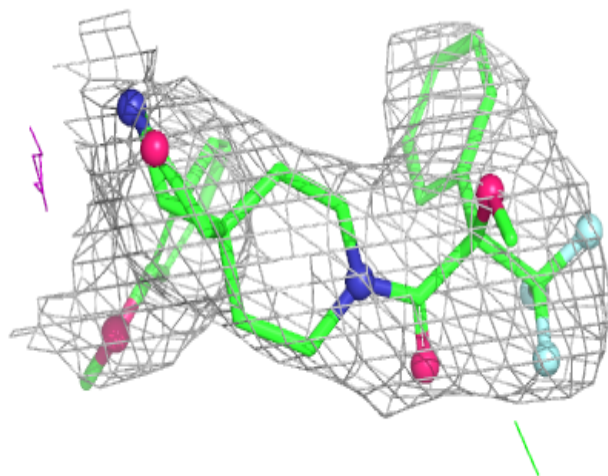
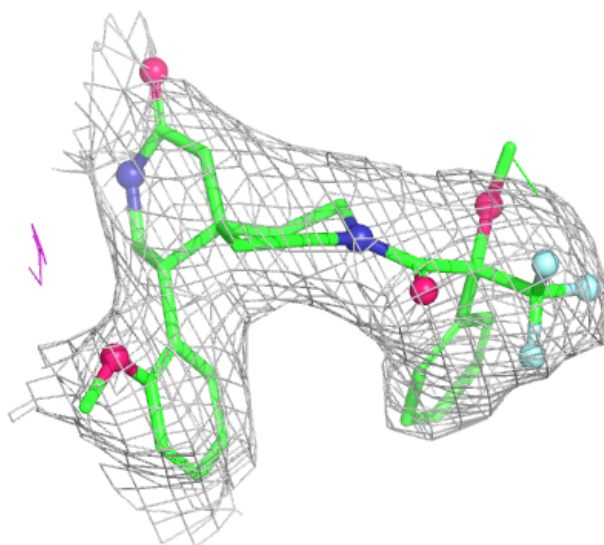
Electron density around A1HZ4 H 404:

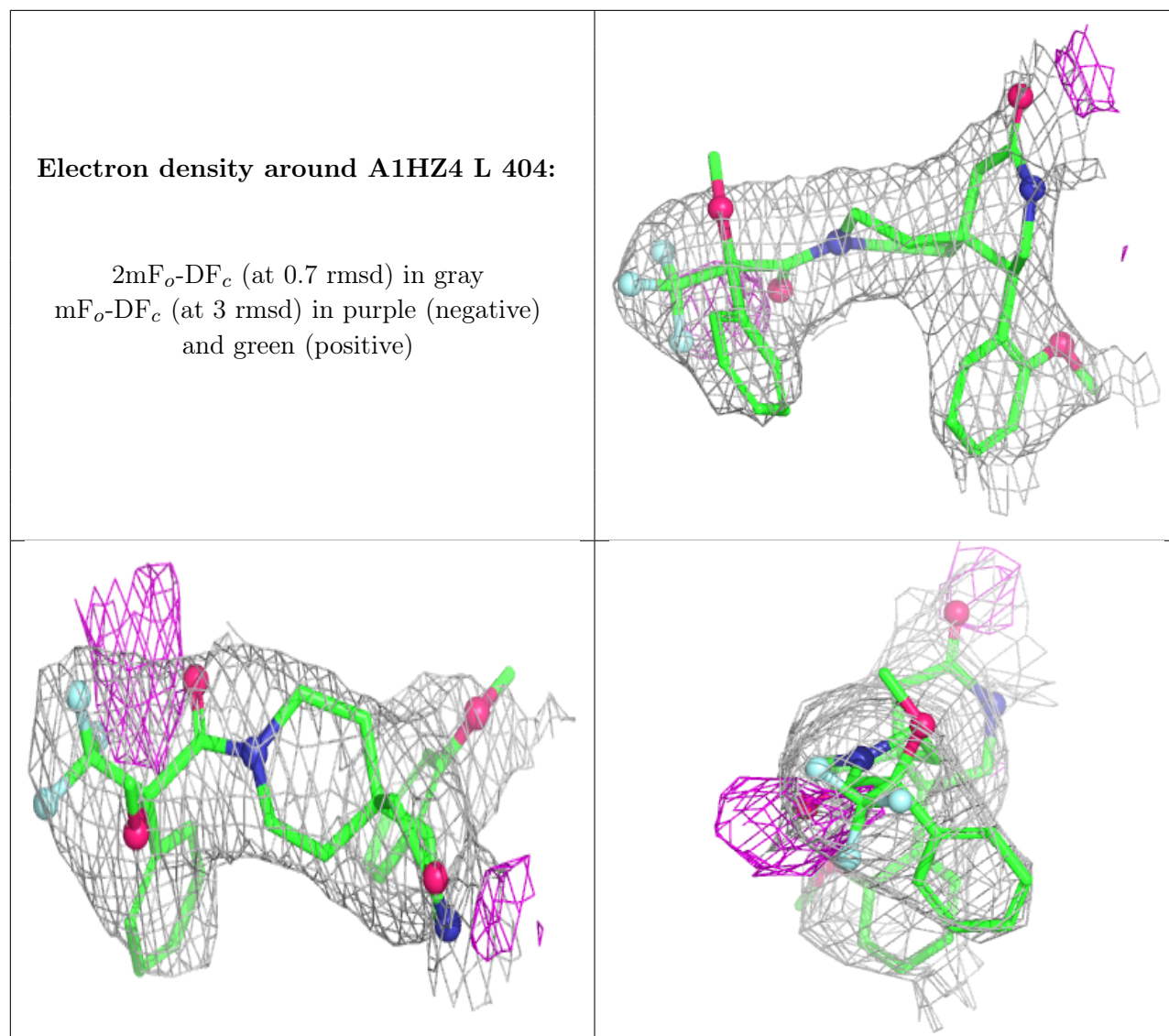
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1HZ4 J 404:

$2mF_o-DF_c$ (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.