WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 01:02 PM EDT

PDB ID	:	4S1D
Title	:	Structure of IgG1 Fab fragment in complex with Biotincytidinamide
Authors	:	Dengl, S.; Hoffmann, E.; Grote, M.; Wagner, C.; Mundigl, O.; Georges, G.; Theorey, I.; Stubenrauch, K.-G.; Bujotzek, A.; Josel, H.-P.; Dziadek, S.; Benz, J.; Brinkmann, U.
Deposited on	:	2015-01-13
Resolution	:	2.50 Å(reported)

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

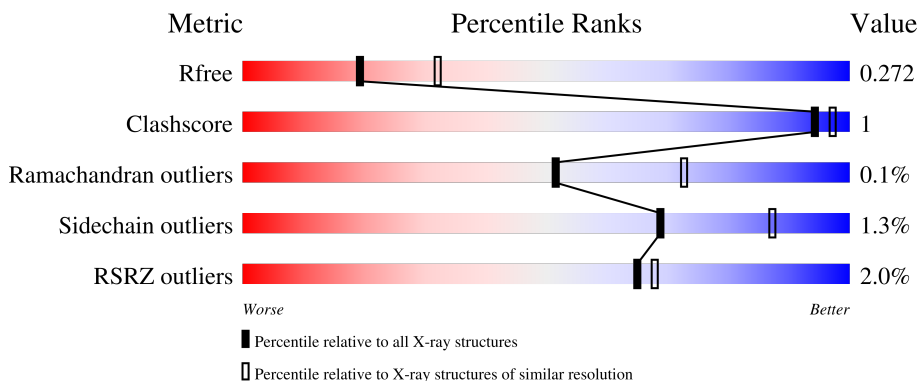|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.50 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.
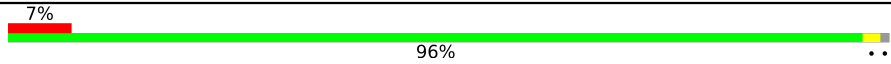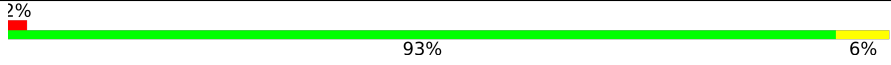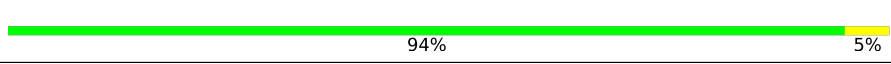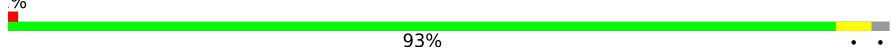
Metric	Percentile Ranks	Value
Rfree		0.272
Clashscore		1
Ramachandran outliers		0.1%
Sidechain outliers		1.3%
RSRZ outliers		2.0%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 <=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	C	220	% 94% · ·
1	E	220	3% 93% 5% ·
1	H	220	95% · ·
1	O	220	% 92% 5% ·

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Mol	Chain	Length	Quality of chain
2	D	214	7% ... 96%
2	F	214	2% ... 93% ... 6%
2	L	214	94% ... 5%
2	P	214	% ... 93% ...

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 13550 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.
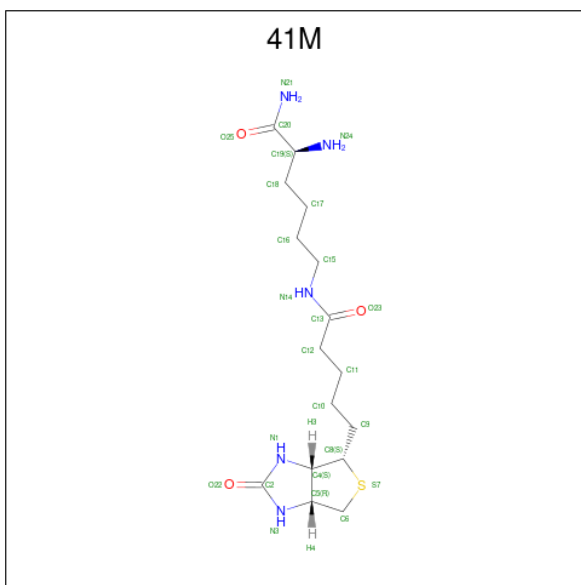
- Molecule 1 is a protein called MAB M33 FAB FRAGMENT, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	216	Total 1650	C 1052	N 268	O 325	S 5	0	0	0
1	C	212	Total 1623	C 1038	N 263	O 317	S 5	0	0	0
1	E	214	Total 1633	C 1043	N 263	O 322	S 5	0	0	0
1	O	213	Total 1632	C 1043	N 264	O 320	S 5	0	0	0

- Molecule 2 is a protein called MAB M33 FAB FRAGMENT, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total 1654	C 1033	N 279	O 336	S 6	0	0	0
2	D	211	Total 1637	C 1024	N 276	O 331	S 6	0	0	0
2	F	213	Total 1654	C 1033	N 279	O 336	S 6	0	0	0
2	P	210	Total 1626	C 1018	N 272	O 330	S 6	0	0	0

- Molecule 3 is N 6 -{5-[(3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanoyl}-L-lysinamide (three-letter code: 41M) (formula: $C_{16}H_{29}N_5O_3S$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	H	1	Total 25	C 16	N 5	O 3	S 1	0	0
3	D	1	Total 25	C 16	N 5	O 3	S 1	0	0
3	E	1	Total 25	C 16	N 5	O 3	S 1	0	0
3	P	1	Total 25	C 16	N 5	O 3	S 1	0	0

• Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
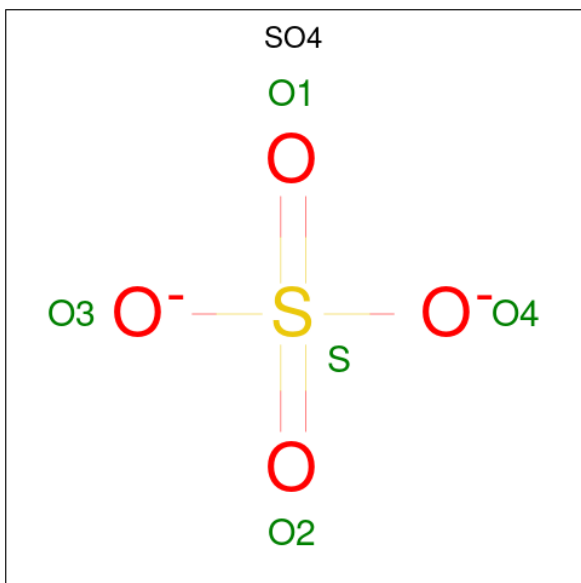
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	O	1	Total 5	O 4	S 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	51	Total 51	O 51	0	0
5	L	46	Total 46	O 46	0	0
5	C	49	Total 49	O 49	0	0
5	D	48	Total 48	O 48	0	0
5	E	22	Total 22	O 22	0	0
5	F	18	Total 18	O 18	0	0
5	O	58	Total 58	O 58	0	0
5	P	44	Total 44	O 44	0	0

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3 Residue-property plots ⓘ

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

• Molecule 1: MAB M33 FAB FRAGMENT, heavy chain
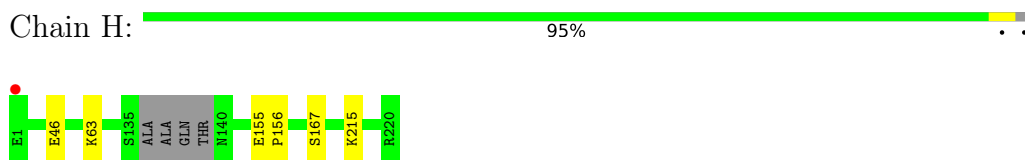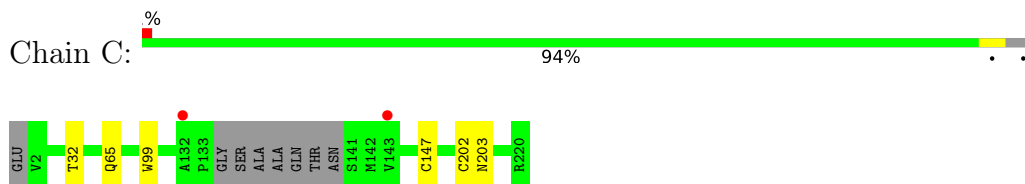
Chain H:

• Molecule 1: MAB M33 FAB FRAGMENT, heavy chain

Chain C:

• Molecule 1: MAB M33 FAB FRAGMENT, heavy chain

Chain E:

• Molecule 1: MAB M33 FAB FRAGMENT, heavy chain

Chain O:

• Molecule 2: MAB M33 FAB FRAGMENT, light chain

Chain L:

• Molecule 2: MAB M33 FAB FRAGMENT, light chain

Chain D:

7%

96%

D1 Q6 C23 Y140 P141 W148 K149 I150 D151 R155 T182 Y186 S191 Y192 E195 A196 S201 P204 I205 V206 F209 N210 R211 ASN GLU CYS

• Molecule 2: MAB M33 FAB FRAGMENT, light chain

Chain F:

2%

93%   6%

D1 Q6 S7 C23 N31 Q37 L47 R61 G68 N76 P80 I106 L125 G128 K149 T193 N212 E213 CYS

• Molecule 2: MAB M33 FAB FRAGMENT, light chain

Chain P:

%

93%

D1 N31 S50 A51 F91 Y96 A130 K147 I150 L179 D184 E195 V206 N210 ARG ASN GLU CYS
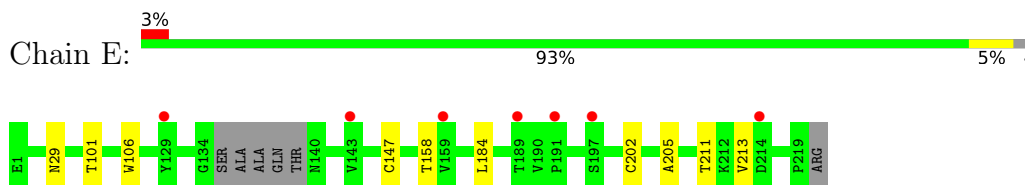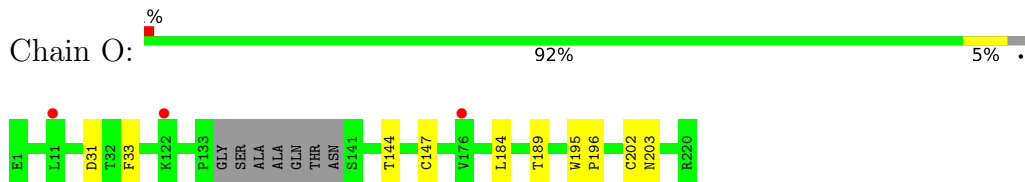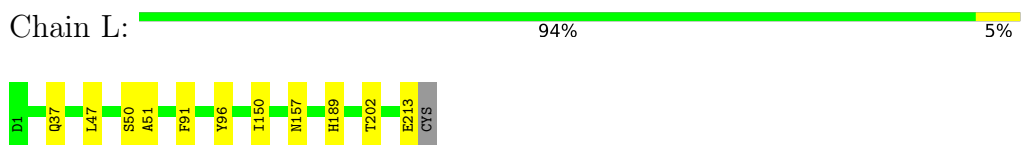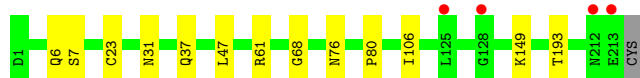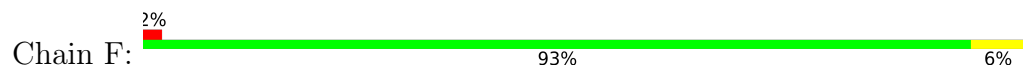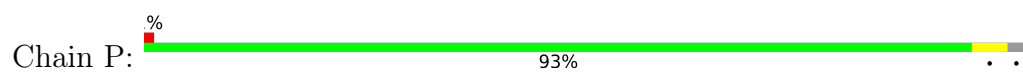
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.09Å 119.62Å 96.18Å 90.00° 117.15° 90.00°	Depositor
Resolution (Å)	119.00 – 2.50 49.02 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (119.00-2.50) 99.9 (49.02-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.225 , 0.274 0.227 , 0.272	Depositor DCC
R_{free} test set	3762 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	57.1	Xtriage
Anisotropy	0.241	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 46.0	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13550	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 41M, SO4

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	C	0.31	0/1669	0.50	0/2287
1	E	0.28	0/1679	0.47	0/2301
1	H	0.31	0/1696	0.52	0/2323
1	O	0.30	0/1678	0.50	0/2299
2	D	0.30	0/1676	0.50	0/2274
2	F	0.28	0/1693	0.46	0/2297
2	L	0.33	0/1693	0.51	0/2297
2	P	0.30	0/1665	0.47	0/2260
All	All	0.30	0/13449	0.49	0/18338

There are no bond length outliers.

There are no bond angle outliers.

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	C	1623	0	1578	1	0
1	E	1633	0	1583	5	0
1	H	1650	0	1601	2	0
1	O	1632	0	1587	7	0
2	D	1637	0	1567	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1654	0	1579	5	0
2	L	1654	0	1579	4	0
2	P	1626	0	1554	5	0
3	D	25	0	29	0	0
3	E	25	0	29	3	0
3	H	25	0	29	0	0
3	P	25	0	29	3	0
4	O	5	0	0	0	0
5	C	49	0	0	0	0
5	D	48	0	0	0	0
5	E	22	0	0	0	0
5	F	18	0	0	0	0
5	H	51	0	0	0	0
5	L	46	0	0	0	0
5	O	58	0	0	1	0
5	P	44	0	0	0	0
All	All	13550	0	12744	33	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 1.

All (33) 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)
3:E:301:41M:H22	3:E:301:41M:N21	1.79	0.94
1:H:46:GLU:OE2	1:H:63:LYS:NZ	2.17	0.78
2:D:6:GLN:HG2	2:D:23:CYS:SG	2.24	0.78
2:P:150:ILE:HD11	2:P:179:LEU:HD21	1.76	0.67
2:F:6:GLN:HG2	2:F:23:CYS:SG	2.39	0.61
1:O:31:ASP:HB2	3:P:301:41M:N24	2.21	0.56
3:E:301:41M:N21	3:E:301:41M:C17	2.63	0.53
1:E:29:ASN:HD22	1:E:101:THR:CG2	2.24	0.50
1:O:31:ASP:HB2	3:P:301:41M:H28	1.76	0.50
2:L:50:SER:O	2:L:51:ALA:HB3	2.12	0.49
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.95	0.49
2:P:50:SER:O	2:P:51:ALA:HB3	2.13	0.48
1:E:158:THR:HB	1:E:205:ALA:HB3	1.96	0.48
1:O:184:LEU:C	1:O:184:LEU:HD12	2.34	0.48
1:O:195:TRP:CG	1:O:196:PRO:HA	2.48	0.48
1:O:144:THR:OG1	1:O:189:THR:HG22	2.17	0.45
1:E:184:LEU:HD12	1:E:184:LEU:C	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:THR:HG21	1:C:99:TRP:O	2.17	0.44
1:E:211:THR:HG22	1:E:213:VAL:HG23	1.99	0.43
1:E:106:TRP:CZ3	3:E:301:41M:H7	2.54	0.43
2:L:91:PHE:HA	2:L:96:TYR:CD1	2.53	0.43
2:P:147:LYS:HB3	2:P:195:GLU:HB2	1.99	0.43
2:F:80:PRO:O	2:F:106:ILE:HD11	2.19	0.43
1:O:33:PHE:CE1	3:P:301:41M:H18	2.54	0.42
2:P:91:PHE:HA	2:P:96:TYR:CD1	2.53	0.42
1:O:189:THR:HG23	5:O:458:HOH:O	2.19	0.42
1:H:155:GLU:HG3	1:H:156:PRO:HA	2.02	0.42
2:P:184:ASP:OD1	2:P:184:ASP:N	2.50	0.42
2:F:149:LYS:HB2	2:F:193:THR:HB	2.02	0.41
2:D:140:TYR:CG	2:D:141:PRO:HA	2.56	0.41
2:L:150:ILE:HD11	2:L:189:HIS:CD2	2.56	0.41
2:F:37:GLN:HB2	2:F:47:LEU:HD11	2.01	0.41
2:F:61:ARG:HB2	2:F:76:ASN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	C	208/220 (94%)	205 (99%)	3 (1%)	0	100	100
1	E	210/220 (96%)	200 (95%)	10 (5%)	0	100	100
1	H	212/220 (96%)	208 (98%)	4 (2%)	0	100	100
1	O	209/220 (95%)	206 (99%)	3 (1%)	0	100	100
2	D	209/214 (98%)	201 (96%)	8 (4%)	0	100	100
2	F	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	29	48
2	L	211/214 (99%)	205 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	208/214 (97%)	196 (94%)	12 (6%)	0	100	100
All	All	1678/1736 (97%)	1624 (97%)	53 (3%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	68	GLY

5.3.2 Protein sidechains ⓘ

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	C	183/188 (97%)	179 (98%)	4 (2%)	52	77
1	E	184/188 (98%)	182 (99%)	2 (1%)	73	89
1	H	186/188 (99%)	184 (99%)	2 (1%)	73	89
1	O	184/188 (98%)	181 (98%)	3 (2%)	62	84
2	D	186/189 (98%)	185 (100%)	1 (0%)	88	96
2	F	188/189 (100%)	186 (99%)	2 (1%)	73	89
2	L	188/189 (100%)	185 (98%)	3 (2%)	62	84
2	P	185/189 (98%)	183 (99%)	2 (1%)	73	89
All	All	1484/1508 (98%)	1465 (99%)	19 (1%)	69	87

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	167	SER
1	H	215	LYS
2	L	157	ASN
2	L	202	THR
2	L	213	GLU
1	C	65	GLN
1	C	147	CYS

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Mol	Chain	Res	Type
1	C	202	CYS
1	C	203	ASN
2	D	151	ASP
1	E	147	CYS
1	E	202	CYS
2	F	7	SER
2	F	31	ASN
1	O	147	CYS
1	O	202	CYS
1	O	203	ASN
2	P	31	ASN
2	P	184	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	31	ASN
1	C	65	GLN
1	C	206	HIS
2	D	145	ASN
1	E	84	ASN
2	F	124	GLN
2	F	156	GLN
2	F	161	ASN
2	F	190	ASN
1	O	28	ASN
1	O	84	ASN
2	P	31	ASN
2	P	76	ASN
2	P	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	41M	E	301	-	26,26,26	0.94	3 (11%)	33,34,34	1.37	3 (9%)
3	41M	D	301	-	26,26,26	0.95	2 (7%)	33,34,34	1.56	4 (12%)
4	SO4	O	301	-	4,4,4	0.34	0	6,6,6	0.40	0
3	41M	P	301	-	26,26,26	0.86	2 (7%)	33,34,34	1.22	4 (12%)
3	41M	H	301	-	26,26,26	0.90	1 (3%)	33,34,34	1.29	2 (6%)

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	41M	H	301	-	-	6/19/40/40	0/2/2/2
3	41M	P	301	-	-	6/19/40/40	0/2/2/2
3	41M	E	301	-	-	12/19/40/40	0/2/2/2
3	41M	D	301	-	-	7/19/40/40	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	41M	C13-N14	2.20	1.38	1.33
3	P	301	41M	C20-N21	2.13	1.38	1.32
3	E	301	41M	C2-N3	2.10	1.38	1.35
3	D	301	41M	C20-N21	2.07	1.38	1.32
3	P	301	41M	C2-N1	2.03	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	301	41M	C20-N21	2.03	1.38	1.32
3	E	301	41M	C20-N21	2.01	1.38	1.32
3	E	301	41M	C2-N1	2.01	1.38	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	41M	C6-C5-N3	-5.91	105.51	113.03
3	E	301	41M	C6-C5-N3	-4.10	107.82	113.03
3	D	301	41M	C10-C9-C8	-3.38	107.00	113.86
3	H	301	41M	C6-C5-N3	-2.93	109.31	113.03
3	P	301	41M	C6-C5-N3	-2.82	109.45	113.03
3	H	301	41M	C5-C6-S7	2.75	108.66	106.31
3	P	301	41M	C10-C9-C8	-2.68	108.42	113.86
3	P	301	41M	O23-C13-N14	-2.36	118.56	123.01
3	D	301	41M	C4-N1-C2	-2.27	110.50	112.62
3	P	301	41M	C4-C5-N3	2.21	104.78	102.43
3	E	301	41M	C10-C9-C8	-2.19	109.42	113.86
3	E	301	41M	O25-C20-N21	-2.04	119.46	123.00
3	D	301	41M	C6-C5-C4	2.02	110.42	108.66

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	41M	C4-C8-C9-C10
3	D	301	41M	S7-C8-C9-C10
3	D	301	41M	C17-C18-C19-C20
3	D	301	41M	C17-C18-C19-N24
3	E	301	41M	C4-C8-C9-C10
3	E	301	41M	S7-C8-C9-C10
3	E	301	41M	C17-C18-C19-C20
3	E	301	41M	C17-C18-C19-N24
3	P	301	41M	N24-C19-C20-N21
3	P	301	41M	N14-C15-C16-C17
3	E	301	41M	N14-C15-C16-C17
3	H	301	41M	C10-C11-C12-C13
3	H	301	41M	N14-C15-C16-C17
3	D	301	41M	C16-C17-C18-C19
3	E	301	41M	C16-C17-C18-C19
3	E	301	41M	C9-C10-C11-C12
3	H	301	41M	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
3	E	301	41M	C15-C16-C17-C18
3	P	301	41M	C15-C16-C17-C18
3	D	301	41M	C9-C10-C11-C12
3	E	301	41M	C11-C12-C13-O23
3	P	301	41M	N24-C19-C20-O25
3	D	301	41M	C15-C16-C17-C18
3	E	301	41M	C11-C12-C13-N14
3	P	301	41M	C18-C19-C20-N21
3	P	301	41M	C18-C19-C20-O25
3	H	301	41M	C17-C18-C19-N24
3	H	301	41M	C11-C10-C9-C8
3	E	301	41M	C18-C19-C20-O25
3	E	301	41M	N24-C19-C20-O25
3	H	301	41M	C15-C16-C17-C18

There are no ring outliers.
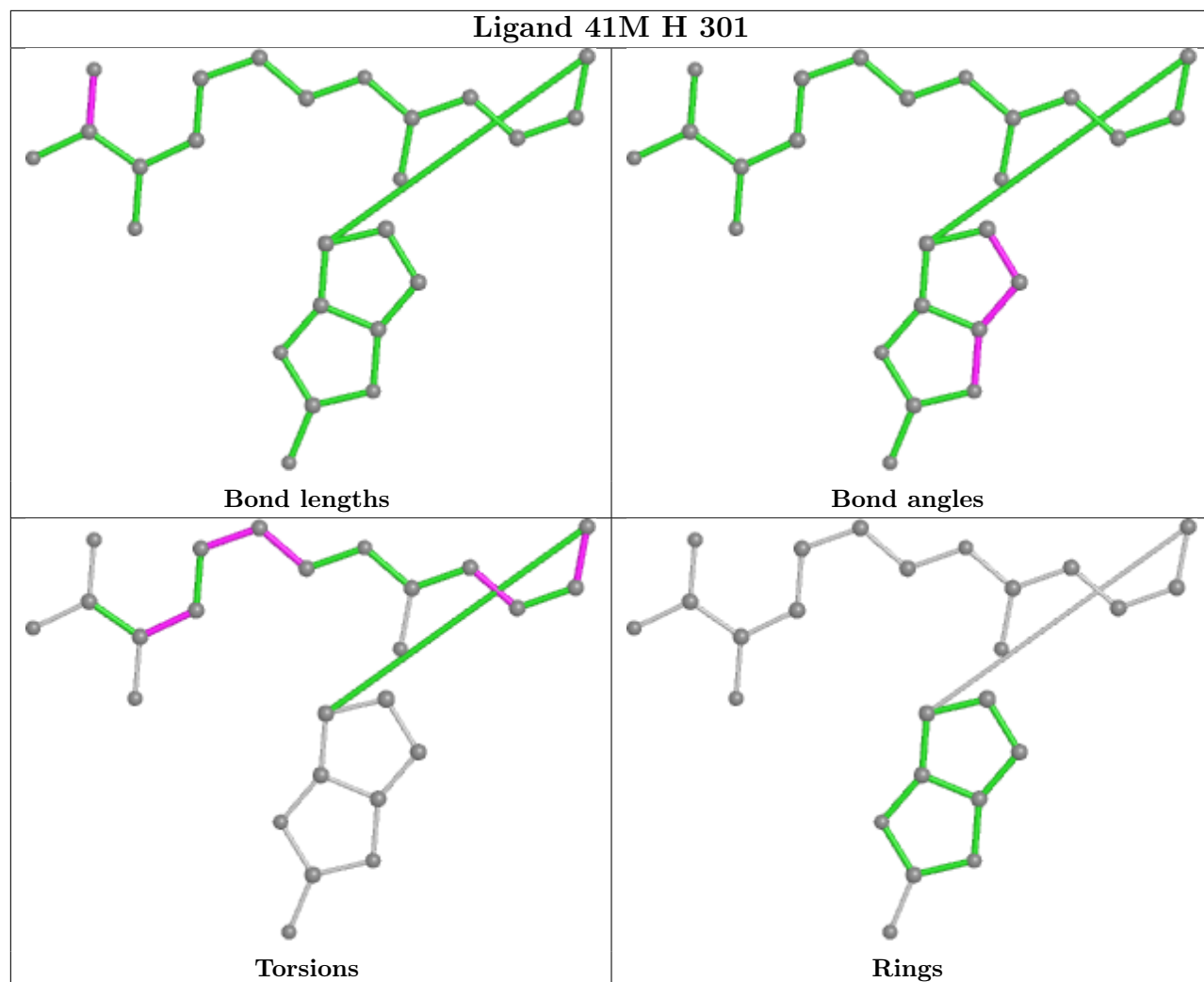
2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	301	41M	3	0
3	P	301	41M	3	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 41M E 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 41M D 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 41M P 301

Bond lengths

Bond angles

Torsions

Rings

Ligand 41M H 301
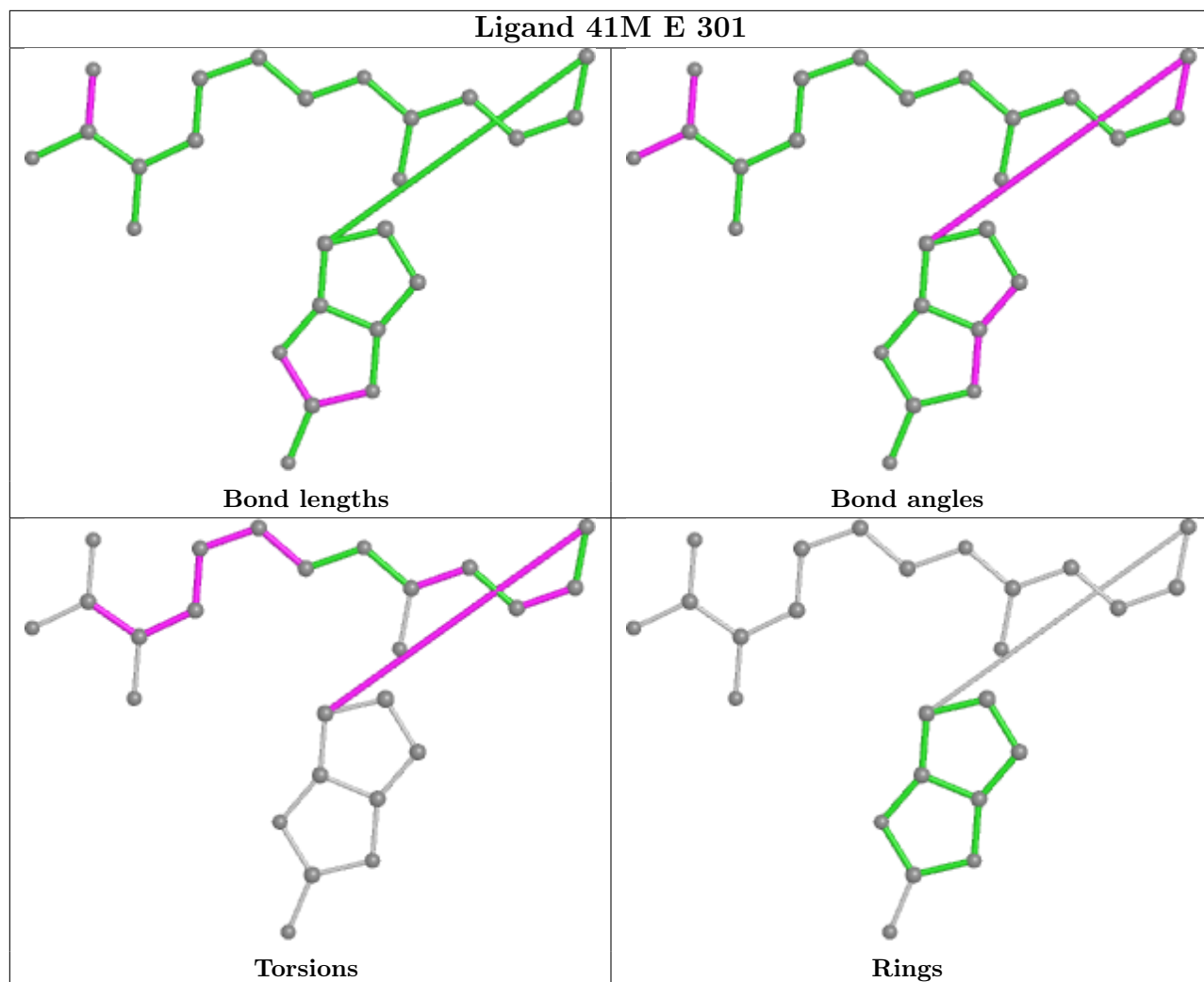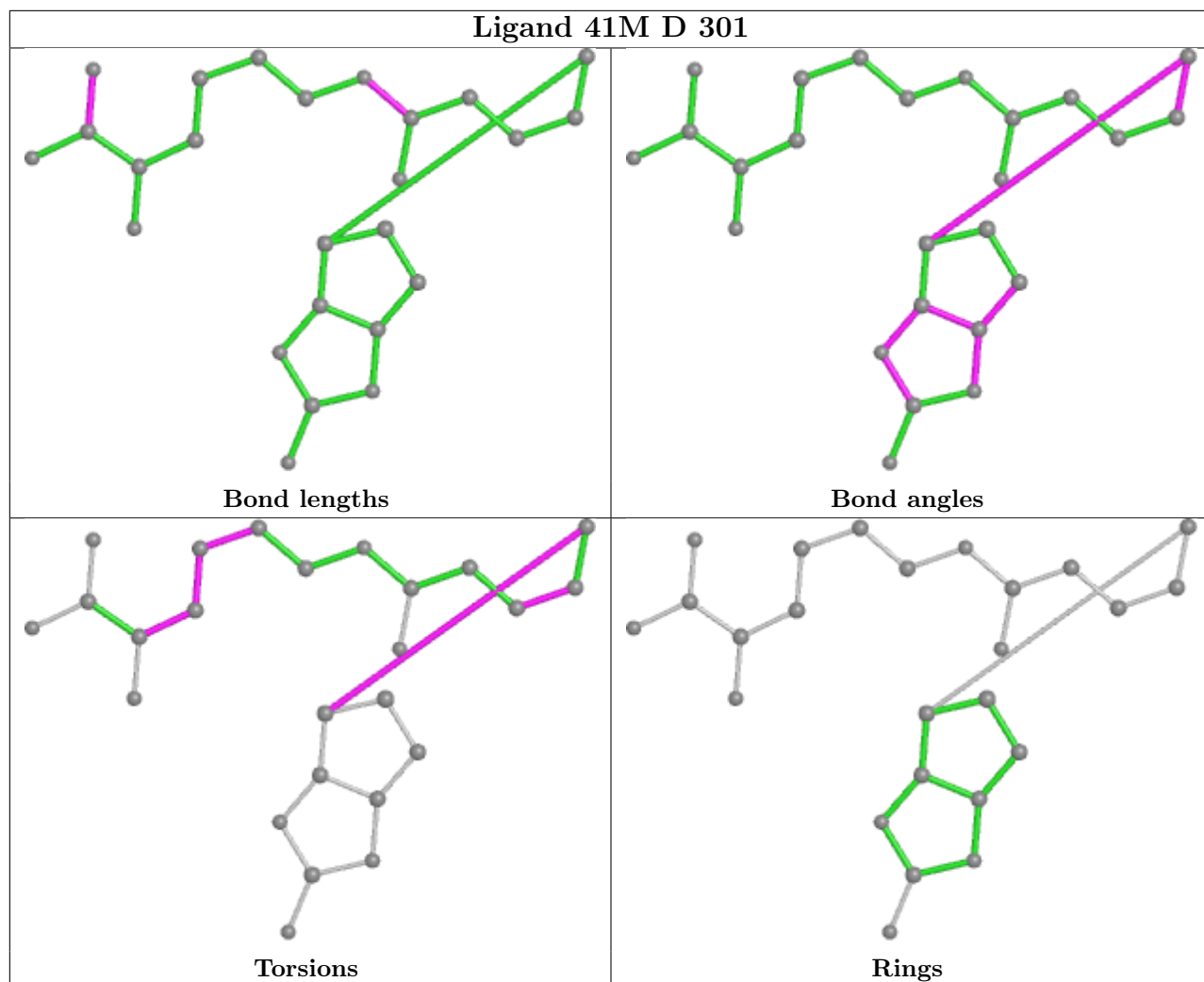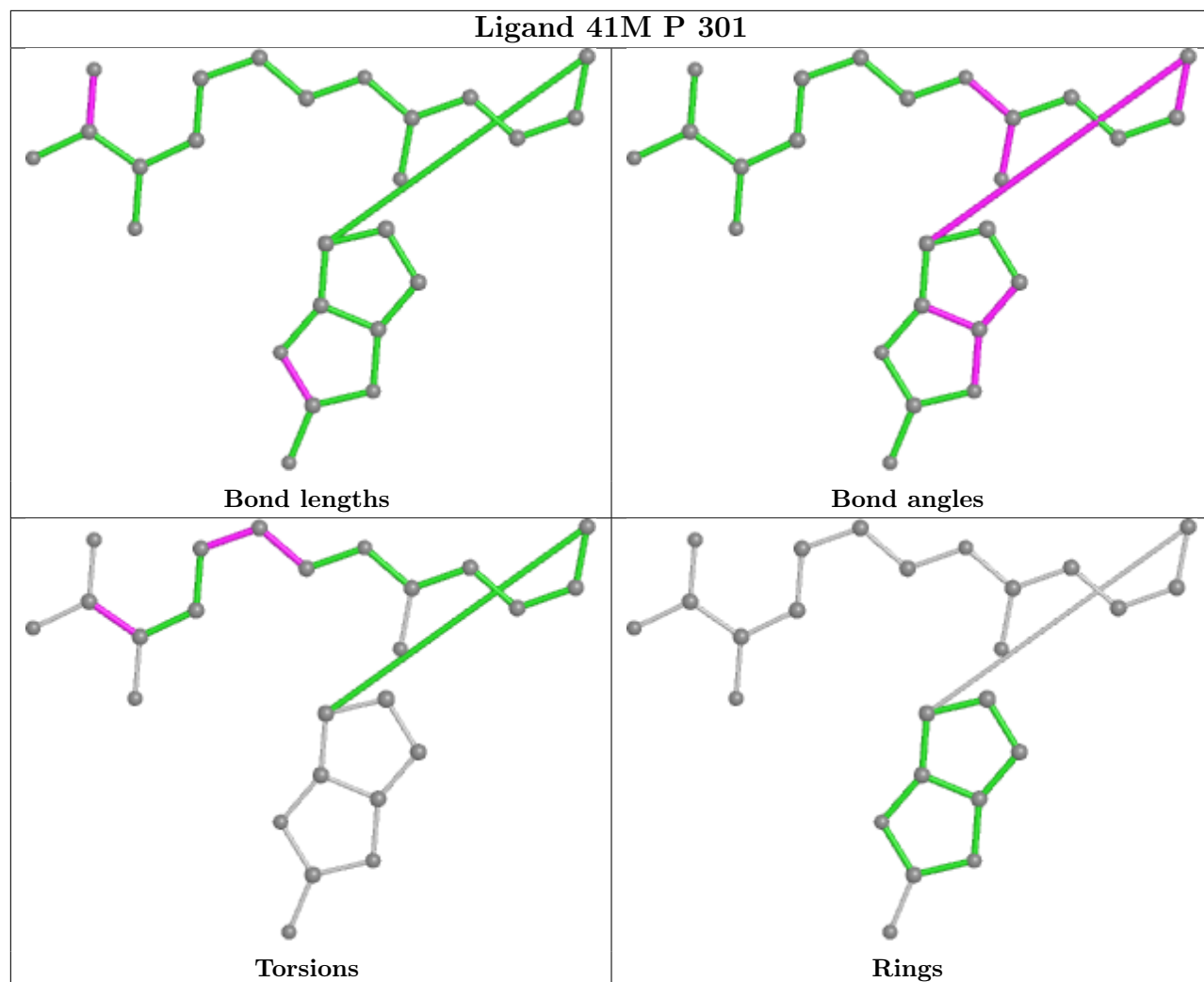
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	C	212/220 (96%)	-0.21	2 (0%)	84	86	46, 76, 106, 121	0
1	E	214/220 (97%)	0.06	7 (3%)	46	50	62, 91, 116, 145	0
1	H	216/220 (98%)	-0.19	1 (0%)	91	91	50, 63, 81, 101	0
1	O	213/220 (96%)	-0.07	3 (1%)	75	77	43, 79, 112, 123	0
2	D	211/214 (98%)	0.16	14 (6%)	18	19	47, 77, 154, 166	0
2	F	213/214 (99%)	-0.03	4 (1%)	66	69	70, 94, 122, 150	0
2	L	213/214 (99%)	-0.15	0	100	100	53, 69, 85, 91	0
2	P	210/214 (98%)	-0.07	3 (1%)	75	77	49, 78, 116, 125	0
All	All	1702/1736 (98%)	-0.06	34 (1%)	65	68	43, 78, 119, 166	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	191	SER	5.5
2	D	206	VAL	4.4
2	D	209	PHE	4.2
2	D	155	ARG	3.9
2	D	186	TYR	3.5
2	D	182	THR	3.3
2	F	213	GLU	3.0
2	D	201	SER	2.9
1	O	122	LYS	2.7
1	E	197	SER	2.7
2	D	192	TYR	2.6
2	P	210	ASN	2.5
2	F	125	LEU	2.5
2	P	206	VAL	2.5
2	D	149	LYS	2.5
1	E	143	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	204	PRO	2.4
1	C	132	ALA	2.4
2	D	196	ALA	2.4
1	C	143	VAL	2.3
1	E	191	PRO	2.3
2	P	130	ALA	2.3
1	O	11	LEU	2.3
1	H	1	GLU	2.2
2	F	212	ASN	2.2
2	F	128	GLY	2.2
1	O	176	VAL	2.1
1	E	189	THR	2.1
2	D	148	TRP	2.0
1	E	129	TYR	2.0
2	D	150	ILE	2.0
1	E	214	ASP	2.0
1	E	159	VAL	2.0
2	D	195	GLU	2.0

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 monosaccharides 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($Å^2$)	Q<0.9
3	41M	E	301	25/25	0.93	0.15	66,74,85,86	0
3	41M	D	301	25/25	0.94	0.20	55,61,83,84	0
3	41M	H	301	25/25	0.94	0.18	53,61,94,97	0
3	41M	P	301	25/25	0.95	0.17	41,51,82,87	0
4	SO4	O	301	5/5	0.96	0.14	55,57,61,67	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.
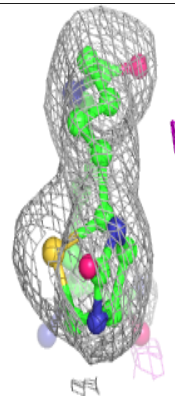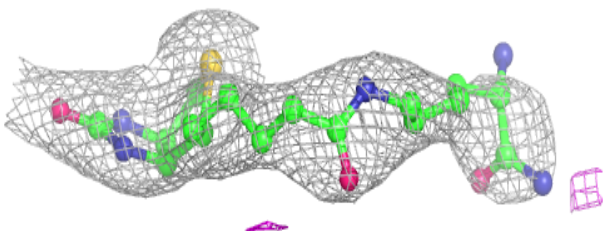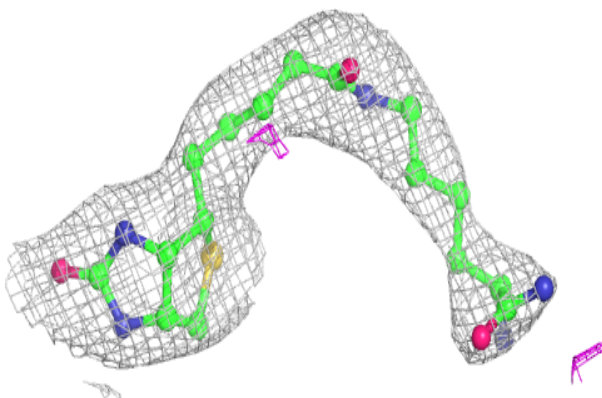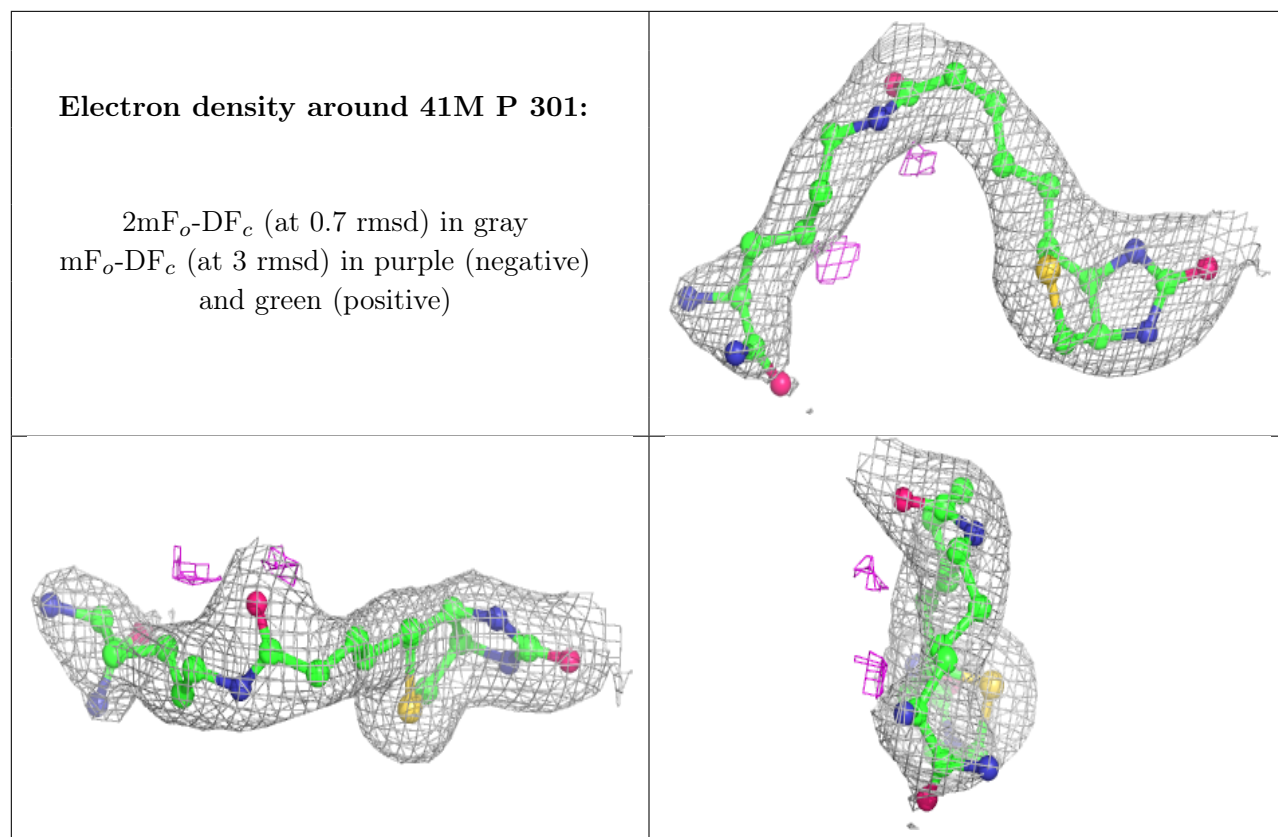
Electron density around 41M E 301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)
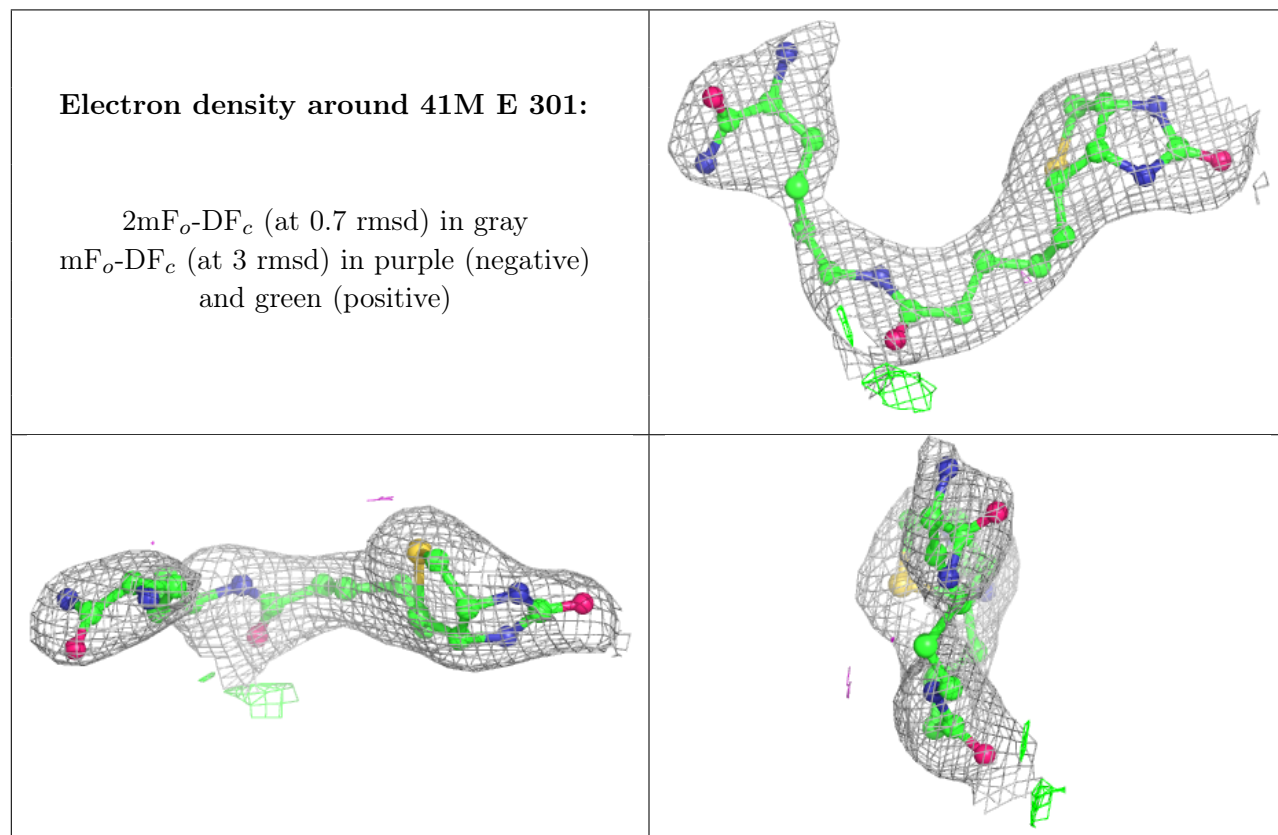
Electron density around 41M D 301:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
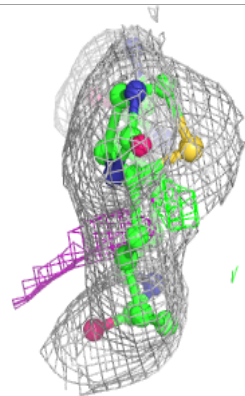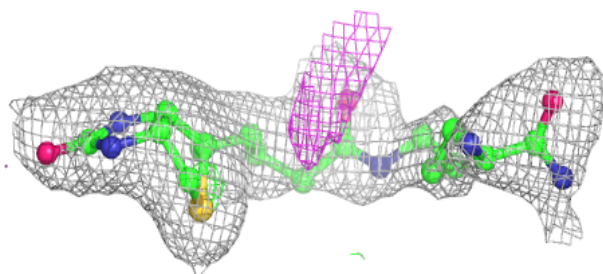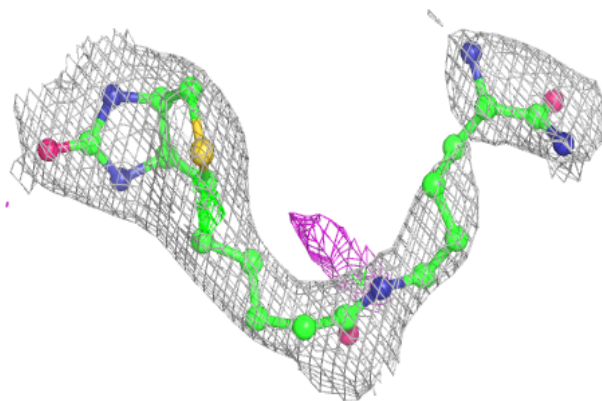
Electron density around 41M H 301:

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

Electron density around 41M P 301:

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.