



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 09:06 AM EDT

PDB ID : 6SQ8
Title : Structure of amide bond synthetase McbA from Marinactinospora thermotolerans
Authors : Rowlinson, B.; Petchey, M.; Grogan, G.
Deposited on : 2019-09-03
Resolution : 2.59 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

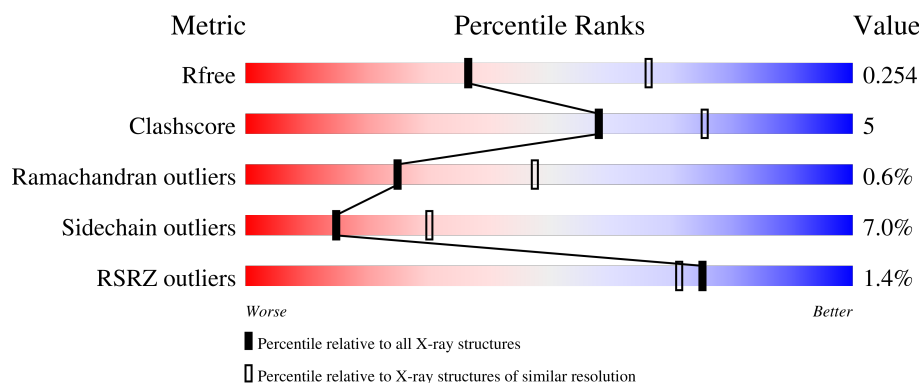
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	498	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	498	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>...</div> </div> </div>
1	C	498	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	498	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div> </div>
1	E	498	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18672 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.

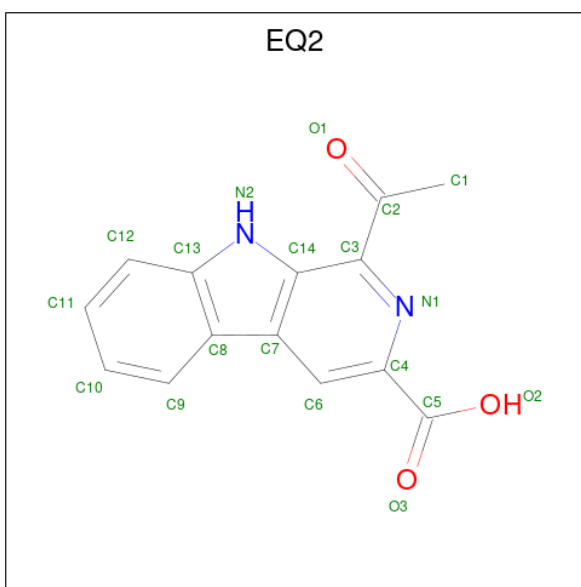
- Molecule 1 is a protein called Fatty acid CoA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3579	2264	643	659	13			
1	B	494	Total	C	N	O	S	0	0	0
			3634	2295	654	672	13			
1	C	489	Total	C	N	O	S	0	2	0
			3615	2282	654	666	13			
1	D	487	Total	C	N	O	S	0	0	0
			3584	2262	650	659	13			
1	E	494	Total	C	N	O	S	0	0	0
			3594	2269	651	662	12			

There are 15 discrepancies between the modelled and reference sequences:

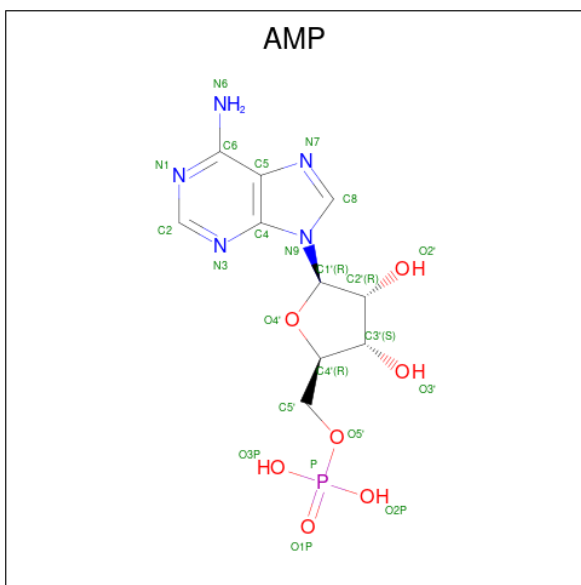
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP R4R1U5
A	-1	PRO	-	expression tag	UNP R4R1U5
A	0	ALA	-	expression tag	UNP R4R1U5
B	-2	GLY	-	expression tag	UNP R4R1U5
B	-1	PRO	-	expression tag	UNP R4R1U5
B	0	ALA	-	expression tag	UNP R4R1U5
C	-2	GLY	-	expression tag	UNP R4R1U5
C	-1	PRO	-	expression tag	UNP R4R1U5
C	0	ALA	-	expression tag	UNP R4R1U5
D	-2	GLY	-	expression tag	UNP R4R1U5
D	-1	PRO	-	expression tag	UNP R4R1U5
D	0	ALA	-	expression tag	UNP R4R1U5
E	-2	GLY	-	expression tag	UNP R4R1U5
E	-1	PRO	-	expression tag	UNP R4R1U5
E	0	ALA	-	expression tag	UNP R4R1U5

- Molecule 2 is 1-ethanoyl-9 {H}-pyrido[3,4-b]indole-3-carboxylic acid (three-letter code: EQ2) (formula: C₁₄H₁₀N₂O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			19	14	2	3		
2	B	1	Total	C	N	O	0	0
			19	14	2	3		
2	C	1	Total	C	N	O	0	0
			19	14	2	3		
2	D	1	Total	C	N	O	0	0
			19	14	2	3		
2	E	1	Total	C	N	O	0	0
			19	14	2	3		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	D	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O		0	0
			19	10	5	4			

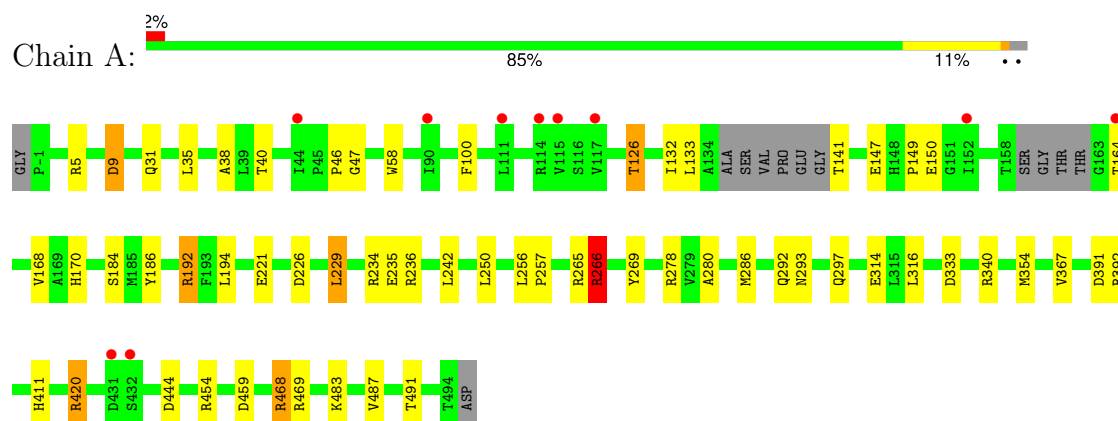
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	89	Total	O	0	0
			89	89		
4	C	101	Total	O	0	0
			101	101		
4	D	99	Total	O	0	0
			99	99		
4	E	66	Total	O	0	0
			66	66		

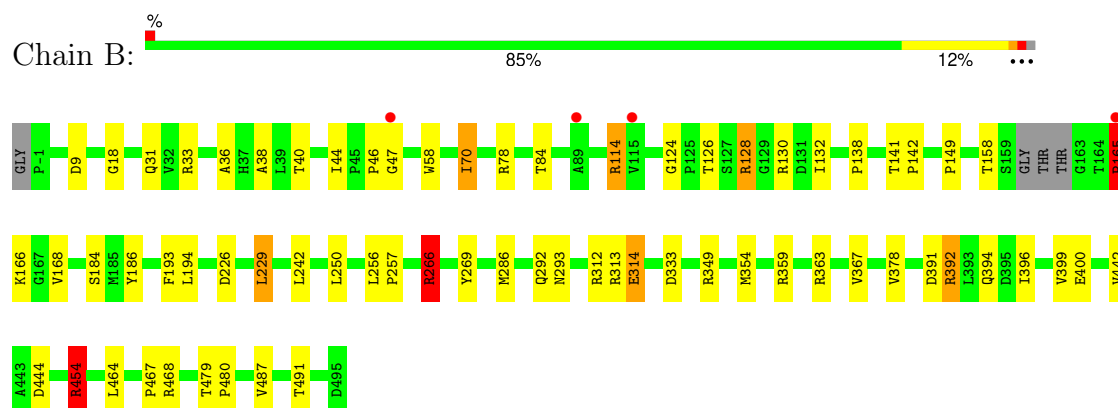
3 Residue-property plots

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.

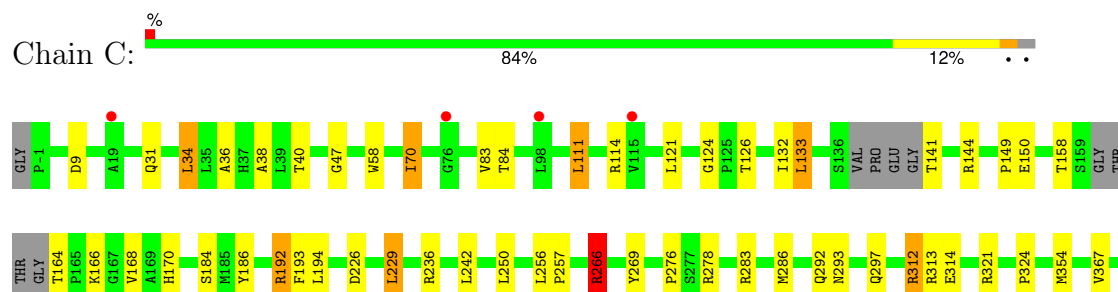
• Molecule 1: Fatty acid CoA ligase

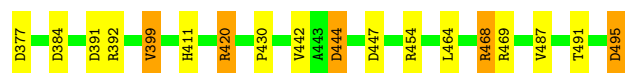


• Molecule 1: Fatty acid CoA ligase

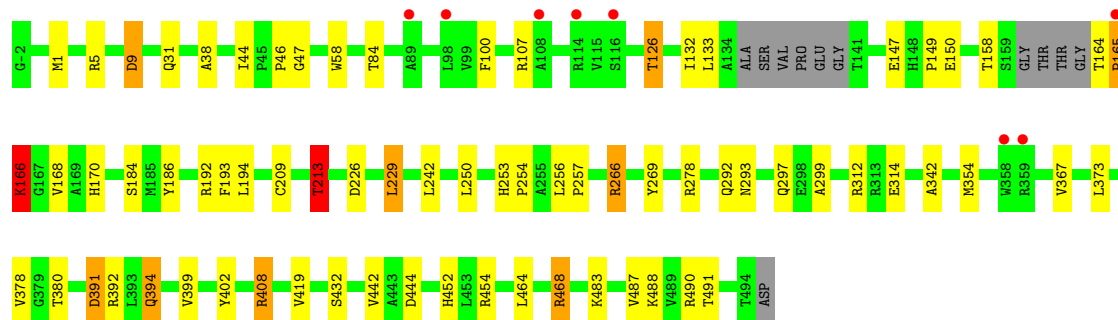
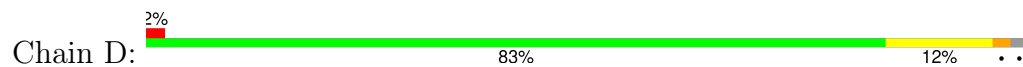


• Molecule 1: Fatty acid CoA ligase

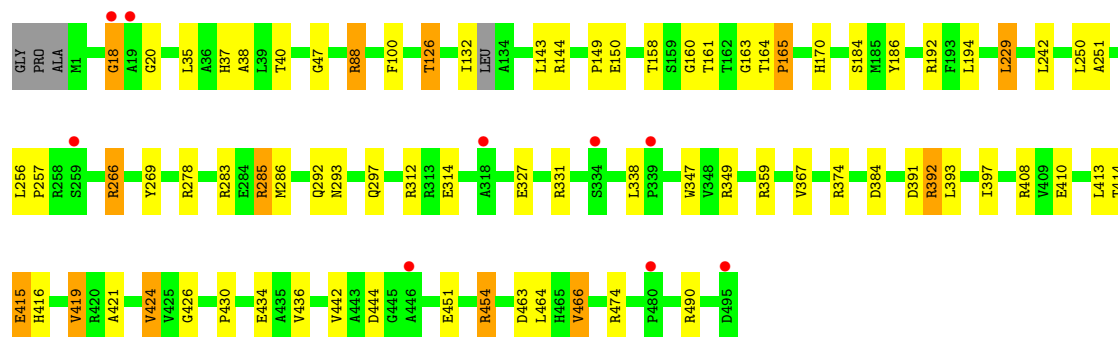
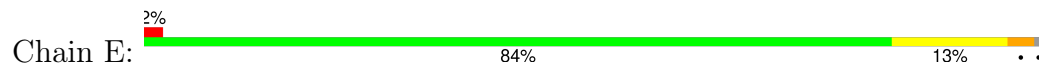




• Molecule 1: Fatty acid CoA ligase



• Molecule 1: Fatty acid CoA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.08Å 131.03Å 196.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.54 – 2.59 65.54 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.9 (65.54-2.59) 99.9 (65.54-2.59)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.213 , 0.249 0.216 , 0.254	Depositor DCC
R_{free} test set	4768 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18672	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, EQ2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/3660	0.68	0/5009
1	B	0.52	0/3717	0.71	1/5089 (0.0%)
1	C	0.53	0/3702	0.72	0/5065
1	D	0.53	0/3664	0.72	2/5014 (0.0%)
1	E	0.52	0/3676	0.73	0/5038
All	All	0.52	0/18419	0.71	3/25215 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	8
1	C	0	5
1	D	0	5
1	E	0	9
All	All	0	33

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	THR	N-CA-CB	-5.69	99.48	110.30
1	D	408	ARG	CG-CD-NE	5.22	122.77	111.80
1	B	165	PRO	N-CA-CB	-5.04	97.06	102.60

There are no chirality outliers.

All (33) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	236	ARG	Sidechain
1	A	266	ARG	Sidechain
1	A	340	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	468	ARG	Sidechain
1	A	469	ARG	Sidechain
1	B	128	ARG	Sidechain
1	B	266	ARG	Sidechain
1	B	312	ARG	Sidechain
1	B	33	ARG	Sidechain
1	B	359	ARG	Sidechain
1	B	454	ARG	Sidechain
1	B	468	ARG	Sidechain
1	B	78	ARG	Sidechain
1	C	114	ARG	Sidechain
1	C	236	ARG	Sidechain
1	C	266	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	468	ARG	Sidechain
1	D	192	ARG	Sidechain
1	D	312	ARG	Sidechain
1	D	408	ARG	Sidechain
1	D	468	ARG	Sidechain
1	D	490	ARG	Sidechain
1	E	266	ARG	Sidechain
1	E	283	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	359	ARG	Sidechain
1	E	374	ARG	Sidechain
1	E	392	ARG	Sidechain
1	E	454	ARG	Sidechain
1	E	474	ARG	Sidechain
1	E	88	ARG	Sidechain

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	3579	0	3522	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3634	0	3574	35	0
1	C	3615	0	3558	38	0
1	D	3584	0	3525	36	0
1	E	3594	0	3513	34	0
2	A	19	0	0	0	0
2	B	19	0	0	0	0
2	C	19	0	0	2	0
2	D	19	0	0	0	0
2	E	19	0	0	0	0
3	A	23	0	12	5	0
3	B	23	0	12	4	0
3	C	23	0	12	3	0
3	D	23	0	12	4	0
3	E	19	0	12	0	0
4	A	105	0	0	4	0
4	B	89	0	0	4	0
4	C	101	0	0	1	0
4	D	99	0	0	2	0
4	E	66	0	0	1	0
All	All	18672	0	17752	173	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 5.

All (173) 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:C:192:ARG:HH11	1:C:192:ARG:HG2	1.23	1.01
1:B:392:ARG:NH1	3:B:502:AMP:O3'	2.08	0.86
1:D:168:VAL:HG13	1:D:354:MET:HE3	1.59	0.85
4:A:701:HOH:O	1:B:349:ARG:CD	2.23	0.85
1:A:392:ARG:NH1	3:A:502:AMP:O3'	2.14	0.81
1:E:463:ASP:O	1:E:466:VAL:HG12	1.83	0.80
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.46	0.79
1:D:394:GLN:HG2	4:D:652:HOH:O	1.85	0.76
1:C:36:ALA:O	1:C:70:ILE:HD11	1.88	0.74
1:B:114:ARG:HH21	1:B:114:ARG:HG3	1.52	0.74
1:D:419:VAL:O	4:D:601:HOH:O	2.05	0.74
1:E:410:GLU:HG3	1:E:424:VAL:HG13	1.69	0.73
1:E:463:ASP:O	1:E:466:VAL:CG1	2.38	0.71
1:A:221:GLU:CB	4:A:686:HOH:O	2.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:354:MET:HE3	1.74	0.69
1:C:168:VAL:HG13	1:C:354:MET:HE3	1.75	0.69
1:C:229:LEU:HD13	1:C:250:LEU:HD11	1.76	0.67
1:B:18:GLY:O	4:B:601:HOH:O	2.12	0.67
2:C:501:EQ2:O2	3:C:502:AMP:O3P	2.11	0.67
1:A:229:LEU:HD13	1:A:250:LEU:HD11	1.78	0.66
1:C:36:ALA:O	1:C:70:ILE:CD1	2.44	0.66
1:E:397:ILE:HG12	1:E:426:GLY:HA3	1.79	0.65
1:E:327:GLU:OE2	1:E:349:ARG:HD2	1.96	0.65
1:C:392:ARG:NH1	3:C:502:AMP:O3'	2.31	0.64
1:B:168:VAL:HG13	1:B:354:MET:HE3	1.79	0.64
1:D:483:LYS:HE2	3:D:502:AMP:O5'	1.98	0.64
1:B:454:ARG:HD2	1:B:467:PRO:O	1.98	0.63
1:B:229:LEU:HD13	1:B:250:LEU:HD11	1.80	0.63
1:C:192:ARG:HG2	1:C:192:ARG:NH1	2.03	0.61
1:A:31:GLN:HE22	1:A:133:LEU:HD22	1.65	0.61
1:E:229:LEU:HD13	1:E:250:LEU:HD11	1.82	0.61
1:B:479:THR:CG2	1:B:480:PRO:HD2	2.30	0.61
1:B:114:ARG:HH21	1:B:114:ARG:CG	2.13	0.61
1:D:256:LEU:HB3	1:D:257:PRO:HD3	1.84	0.59
1:E:256:LEU:HB3	1:E:257:PRO:HD3	1.84	0.59
1:D:392:ARG:NH1	3:D:502:AMP:O3'	2.35	0.58
1:E:18:GLY:O	1:E:20:GLY:N	2.36	0.58
1:E:392:ARG:NH2	1:E:434:GLU:OE1	2.34	0.58
1:B:479:THR:HG23	1:B:480:PRO:HD2	1.85	0.57
1:D:483:LYS:HE3	3:D:502:AMP:O4'	2.03	0.57
1:E:251:ALA:O	1:E:285:ARG:HD3	2.05	0.57
1:E:35:LEU:HD23	1:E:132:ILE:HG21	1.87	0.57
1:D:168:VAL:HG13	1:D:354:MET:CE	2.33	0.57
1:E:278:ARG:NH2	1:E:430:PRO:O	2.38	0.56
1:C:454:ARG:NH1	1:C:468:ARG:O	2.38	0.56
1:A:454:ARG:NH1	1:A:468:ARG:O	2.38	0.56
1:D:454:ARG:NH1	1:D:468:ARG:O	2.39	0.56
1:A:483:LYS:HE2	3:A:502:AMP:O5'	2.06	0.55
1:B:138:PRO:HB2	1:B:141:THR:OG1	2.07	0.55
1:B:392:ARG:HD3	3:B:502:AMP:O3'	2.08	0.54
1:D:186:TYR:HA	1:D:266:ARG:HD3	1.89	0.54
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.17	0.54
1:C:34:LEU:HD12	1:C:34:LEU:C	2.28	0.54
1:E:414:THR:HA	1:E:419:VAL:HG22	1.91	0.53
1:E:416:HIS:HB3	1:E:419:VAL:HG13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:ARG:NH2	1:C:420[A]:ARG:HD3	2.24	0.53
1:D:209:CYS:O	1:D:213:THR:HB	2.08	0.53
1:E:143:LEU:HD23	1:E:144:ARG:N	2.24	0.53
1:D:158:THR:HG22	1:D:165:PRO:O	2.10	0.52
1:B:158:THR:HB	1:B:165:PRO:O	2.09	0.52
1:D:483:LYS:CE	3:D:502:AMP:O4'	2.58	0.52
1:C:70:ILE:HG23	1:C:70:ILE:O	2.11	0.52
1:D:31:GLN:HG3	1:D:58:TRP:CH2	2.45	0.51
1:E:415:GLU:HA	1:E:415:GLU:OE1	2.09	0.51
1:B:314:GLU:CG	4:B:666:HOH:O	2.58	0.51
1:B:31:GLN:HG3	1:B:58:TRP:CH2	2.46	0.51
1:E:451:GLU:OE2	1:E:454:ARG:NH1	2.39	0.51
1:D:1:MET:HG2	1:D:147:GLU:OE2	2.10	0.51
1:D:229:LEU:HD13	1:D:250:LEU:HD11	1.93	0.51
1:B:454:ARG:CD	1:B:467:PRO:O	2.58	0.51
1:C:321:ARG:NH1	1:C:384:ASP:O	2.43	0.51
1:E:312:ARG:NH2	1:E:384:ASP:OD2	2.40	0.50
1:D:38:ALA:CB	1:D:132:ILE:HG23	2.42	0.50
1:C:469:ARG:NH2	1:C:495:ASP:HB2	2.26	0.50
1:C:31:GLN:HG3	1:C:58:TRP:CH2	2.47	0.49
1:C:124:GLY:N	1:C:133:LEU:HD22	2.27	0.49
1:C:293:ASN:HB3	2:C:501:EQ2:C1	2.42	0.49
1:E:242:LEU:O	1:E:269:TYR:HA	2.13	0.49
1:E:331:ARG:HD2	1:E:347:TRP:CD1	2.47	0.49
1:E:397:ILE:HG12	1:E:426:GLY:CA	2.41	0.49
1:A:242:LEU:O	1:A:269:TYR:HA	2.13	0.49
1:C:242:LEU:O	1:C:269:TYR:HA	2.13	0.49
1:A:31:GLN:HG3	1:A:58:TRP:CH2	2.48	0.48
1:C:38:ALA:HB1	1:C:132:ILE:HG23	1.95	0.48
1:C:121:LEU:HB3	1:C:132:ILE:CG1	2.44	0.48
1:D:242:LEU:O	1:D:269:TYR:HA	2.13	0.48
1:B:242:LEU:O	1:B:269:TYR:HA	2.14	0.48
1:C:283:ARG:NH2	4:C:606:HOH:O	2.47	0.48
1:B:38:ALA:CB	1:B:132:ILE:HG23	2.43	0.48
1:B:124:GLY:O	1:B:126:THR:HG23	2.14	0.48
1:C:38:ALA:CB	1:C:132:ILE:HG23	2.44	0.48
1:B:114:ARG:CG	1:B:114:ARG:NH2	2.77	0.48
1:D:342:ALA:O	1:D:380:THR:OG1	2.17	0.48
1:E:158:THR:O	1:E:158:THR:HG23	2.14	0.48
1:B:47:GLY:HA2	1:B:149:PRO:HD2	1.96	0.47
1:B:130:ARG:HD2	4:B:634:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:ARG:HH11	1:E:192:ARG:HG3	1.80	0.47
1:A:147:GLU:HG3	1:D:402:TYR:OH	2.15	0.47
1:A:38:ALA:CB	1:A:132:ILE:HG23	2.44	0.46
1:C:186:TYR:OH	1:C:293:ASN:ND2	2.48	0.46
1:D:47:GLY:HA2	1:D:149:PRO:HD2	1.97	0.46
1:A:392:ARG:HH11	3:A:502:AMP:HO3'	1.60	0.46
1:B:399:VAL:HG21	1:B:464:LEU:HD22	1.97	0.46
1:A:47:GLY:HA2	1:A:149:PRO:HD2	1.97	0.46
1:A:31:GLN:HE22	1:A:133:LEU:CD2	2.27	0.46
1:C:269:TYR:CE2	1:C:292:GLN:HG3	2.51	0.46
1:A:5:ARG:HH11	1:D:432:SER:HB3	1.80	0.46
1:B:70:ILE:O	1:B:70:ILE:HG23	2.15	0.45
1:B:487:VAL:O	1:B:491:THR:HG23	2.17	0.45
1:C:47:GLY:HA2	1:C:149:PRO:HD2	1.97	0.45
1:C:229:LEU:HD12	1:C:229:LEU:HA	1.88	0.45
1:D:399:VAL:HG21	1:D:464:LEU:HD22	1.98	0.45
1:D:186:TYR:OH	1:D:293:ASN:ND2	2.48	0.45
1:B:186:TYR:OH	1:B:293:ASN:ND2	2.50	0.45
1:D:269:TYR:CE2	1:D:292:GLN:HG3	2.52	0.45
1:B:186:TYR:HA	1:B:266:ARG:HD3	1.98	0.45
1:B:269:TYR:CE2	1:B:292:GLN:HG3	2.52	0.45
1:B:36:ALA:HB1	1:B:70:ILE:HD13	2.00	0.44
1:D:158:THR:HG21	1:D:166:LYS:HE3	1.98	0.44
1:B:392:ARG:HD3	3:B:502:AMP:HO3'	1.82	0.44
1:E:38:ALA:CB	1:E:132:ILE:HG23	2.48	0.44
1:A:269:TYR:CE2	1:A:292:GLN:HG3	2.53	0.44
1:E:88:ARG:NH2	1:E:163:GLY:O	2.49	0.44
1:B:256:LEU:N	1:B:257:PRO:HD2	2.33	0.44
1:A:186:TYR:OH	1:A:293:ASN:ND2	2.51	0.44
1:A:256:LEU:N	1:A:257:PRO:HD2	2.33	0.44
1:A:35:LEU:HD23	1:A:132:ILE:HG21	1.99	0.43
1:A:483:LYS:HE2	3:A:502:AMP:O4'	2.18	0.43
1:B:36:ALA:HB1	1:B:70:ILE:CD1	2.48	0.43
1:C:399:VAL:HG21	1:C:464:LEU:HD22	2.00	0.43
1:A:487:VAL:O	1:A:491:THR:HG23	2.18	0.43
1:E:47:GLY:HA2	1:E:149:PRO:HD2	1.99	0.43
1:A:186:TYR:HA	1:A:266:ARG:HD3	2.01	0.43
1:E:170:HIS:HE1	1:E:297:GLN:O	2.01	0.43
1:A:100:PHE:CZ	1:A:126:THR:HG21	2.54	0.43
1:C:186:TYR:HA	1:C:266:ARG:HD3	2.00	0.43
1:C:487:VAL:O	1:C:491:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:HIS:HE1	1:D:297:GLN:O	2.02	0.43
1:E:269:TYR:CE2	1:E:292:GLN:HG3	2.54	0.43
1:A:265:ARG:CD	4:E:650:HOH:O	2.67	0.42
1:A:483:LYS:CE	3:A:502:AMP:O4'	2.67	0.42
1:A:459:ASP:OD2	1:C:312:ARG:NH1	2.52	0.42
1:A:234:ARG:NH1	1:A:235:GLU:OE2	2.52	0.42
1:E:186:TYR:OH	1:E:293:ASN:ND2	2.52	0.42
1:C:170:HIS:HE1	1:C:297:GLN:O	2.02	0.42
1:E:143:LEU:HD23	1:E:143:LEU:C	2.39	0.42
1:E:229:LEU:HD12	1:E:229:LEU:HA	1.87	0.42
1:B:314:GLU:HG2	4:B:666:HOH:O	2.18	0.42
1:B:378:VAL:HG21	1:B:396:ILE:HD11	2.01	0.42
3:B:502:AMP:HO3'	3:B:502:AMP:HO2'	1.40	0.41
1:C:256:LEU:N	1:C:257:PRO:HD2	2.34	0.41
1:E:160:GLY:O	1:E:408:ARG:HG3	2.19	0.41
1:C:447:ASP:OD2	1:E:37:HIS:NE2	2.53	0.41
1:D:487:VAL:O	1:D:491:THR:HG23	2.20	0.41
1:D:100:PHE:CZ	1:D:126:THR:HG21	2.56	0.41
1:D:229:LEU:HD12	1:D:229:LEU:HA	1.89	0.41
1:D:299:ALA:HB2	1:D:373:LEU:HD23	2.02	0.41
1:E:100:PHE:CZ	1:E:126:THR:HG21	2.56	0.41
1:B:142:PRO:HA	1:C:430:PRO:O	2.20	0.41
1:C:377:ASP:OD2	3:C:502:AMP:O3'	2.36	0.41
1:A:170:HIS:HE1	1:A:297:GLN:O	2.03	0.41
4:A:671:HOH:O	1:D:452:HIS:HE1	2.03	0.41
1:C:276:PRO:HG2	1:C:411[B]:HIS:ND1	2.35	0.41
1:C:83:VAL:HG23	1:C:111:LEU:CD1	2.50	0.41
1:C:192:ARG:HH11	1:C:192:ARG:CG	2.08	0.41
1:D:253:HIS:HA	1:D:254:PRO:HD3	1.96	0.41
1:A:5:ARG:O	1:A:9:ASP:HB2	2.21	0.40
1:A:5:ARG:NH1	1:D:432:SER:HB3	2.36	0.40
1:D:5:ARG:O	1:D:9:ASP:HB2	2.20	0.40
1:D:378:VAL:HG12	1:D:391:ASP:O	2.21	0.40
1:A:280:ALA:HB2	1:A:316:LEU:HD13	2.02	0.40
1:A:411:HIS:HB3	4:A:660:HOH:O	2.22	0.40
1:C:399:VAL:O	1:C:399:VAL:CG2	2.70	0.40

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	480/498 (96%)	468 (98%)	11 (2%)	1 (0%)	47	71
1	B	490/498 (98%)	476 (97%)	10 (2%)	4 (1%)	19	39
1	C	485/498 (97%)	470 (97%)	13 (3%)	2 (0%)	34	57
1	D	481/498 (97%)	465 (97%)	12 (2%)	4 (1%)	19	39
1	E	490/498 (98%)	473 (96%)	13 (3%)	4 (1%)	19	39
All	All	2426/2490 (97%)	2352 (97%)	59 (2%)	15 (1%)	25	47

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	165	PRO
1	D	165	PRO
1	A	444	ASP
1	B	444	ASP
1	D	444	ASP
1	E	444	ASP
1	C	158	THR
1	C	444	ASP
1	B	44	ILE
1	D	166	LYS
1	E	165	PRO
1	E	421	ALA
1	D	44	ILE
1	B	166	LYS
1	E	18	GLY

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	355/384 (92%)	335 (94%)	20 (6%)	21	42
1	B	362/384 (94%)	336 (93%)	26 (7%)	14	29
1	C	361/384 (94%)	329 (91%)	32 (9%)	9	19
1	D	356/384 (93%)	333 (94%)	23 (6%)	17	34
1	E	353/384 (92%)	328 (93%)	25 (7%)	14	29
All	All	1787/1920 (93%)	1661 (93%)	126 (7%)	15	29

All (126) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	40	THR
1	A	46	PRO
1	A	126	THR
1	A	141	THR
1	A	150	GLU
1	A	164	THR
1	A	184	SER
1	A	192	ARG
1	A	194	LEU
1	A	226	ASP
1	A	229	LEU
1	A	266	ARG
1	A	278	ARG
1	A	286	MET
1	A	314	GLU
1	A	333	ASP
1	A	367	VAL
1	A	391	ASP
1	A	420	ARG
1	B	9	ASP
1	B	40	THR
1	B	46	PRO
1	B	70	ILE
1	B	84	THR
1	B	114	ARG
1	B	128	ARG
1	B	165	PRO

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Mol	Chain	Res	Type
1	B	184	SER
1	B	193	PHE
1	B	194	LEU
1	B	226	ASP
1	B	229	LEU
1	B	266	ARG
1	B	286	MET
1	B	313	ARG
1	B	314	GLU
1	B	333	ASP
1	B	363	ARG
1	B	367	VAL
1	B	391	ASP
1	B	392	ARG
1	B	394	GLN
1	B	400	GLU
1	B	442	VAL
1	B	454	ARG
1	C	9	ASP
1	C	34	LEU
1	C	40	THR
1	C	70	ILE
1	C	84	THR
1	C	111	LEU
1	C	126	THR
1	C	133	LEU
1	C	141	THR
1	C	144	ARG
1	C	150	GLU
1	C	164	THR
1	C	166	LYS
1	C	184	SER
1	C	192	ARG
1	C	193	PHE
1	C	194	LEU
1	C	226	ASP
1	C	229	LEU
1	C	266	ARG
1	C	286	MET
1	C	313	ARG
1	C	314	GLU
1	C	324	PRO

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Mol	Chain	Res	Type
1	C	367	VAL
1	C	391	ASP
1	C	399	VAL
1	C	420[A]	ARG
1	C	420[B]	ARG
1	C	442	VAL
1	C	444	ASP
1	C	495	ASP
1	D	9	ASP
1	D	46	PRO
1	D	84	THR
1	D	107	ARG
1	D	126	THR
1	D	133	LEU
1	D	150	GLU
1	D	164	THR
1	D	166	LYS
1	D	184	SER
1	D	193	PHE
1	D	194	LEU
1	D	213	THR
1	D	226	ASP
1	D	229	LEU
1	D	266	ARG
1	D	278	ARG
1	D	314	GLU
1	D	367	VAL
1	D	391	ASP
1	D	394	GLN
1	D	442	VAL
1	D	488	LYS
1	E	40	THR
1	E	126	THR
1	E	150	GLU
1	E	161	THR
1	E	164	THR
1	E	165	PRO
1	E	184	SER
1	E	194	LEU
1	E	229	LEU
1	E	266	ARG
1	E	286	MET

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Mol	Chain	Res	Type
1	E	314	GLU
1	E	338	LEU
1	E	367	VAL
1	E	391	ASP
1	E	393	LEU
1	E	413	LEU
1	E	415	GLU
1	E	419	VAL
1	E	424	VAL
1	E	436	VAL
1	E	442	VAL
1	E	464	LEU
1	E	466	VAL
1	E	490	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	54	HIS
1	A	170	HIS
1	A	253	HIS
1	A	293	ASN
1	A	386	HIS
1	A	388	HIS
1	A	452	HIS
1	B	54	HIS
1	B	170	HIS
1	B	253	HIS
1	B	293	ASN
1	B	388	HIS
1	B	394	GLN
1	B	460	HIS
1	C	54	HIS
1	C	170	HIS
1	C	253	HIS
1	C	293	ASN
1	C	388	HIS
1	D	54	HIS
1	D	170	HIS
1	D	253	HIS
1	D	293	ASN

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Mol	Chain	Res	Type
1	D	388	HIS
1	D	394	GLN
1	D	411	HIS
1	D	452	HIS
1	E	54	HIS
1	E	253	HIS
1	E	293	ASN
1	E	388	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	AMP	C	502	-	21,25,25	1.09	1 (4%)	23,38,38	1.53	4 (17%)
3	AMP	B	502	-	21,25,25	1.21	2 (9%)	23,38,38	1.81	6 (26%)
3	AMP	D	502	-	21,25,25	1.15	2 (9%)	23,38,38	1.50	3 (13%)
3	AMP	A	502	-	21,25,25	1.10	2 (9%)	23,38,38	1.68	7 (30%)
2	EQ2	E	501	-	20,21,21	1.38	3 (15%)	24,31,31	0.98	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EQ2	A	501	-	20,21,21	1.00	2 (10%)	24,31,31	1.15	2 (8%)
2	EQ2	C	501	-	20,21,21	0.83	0	24,31,31	1.02	2 (8%)
3	AMP	E	502	-	17,21,25	1.35	2 (11%)	17,31,38	1.75	3 (17%)
2	EQ2	B	501	-	20,21,21	0.96	1 (5%)	24,31,31	1.05	2 (8%)
2	EQ2	D	501	-	20,21,21	0.85	1 (5%)	24,31,31	1.17	2 (8%)

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	AMP	C	502	-	-	0/6/26/26	0/3/3/3
3	AMP	B	502	-	-	3/6/26/26	0/3/3/3
3	AMP	D	502	-	-	0/6/26/26	0/3/3/3
3	AMP	A	502	-	-	0/6/26/26	0/3/3/3
2	EQ2	E	501	-	-	4/8/8/8	0/3/3/3
2	EQ2	A	501	-	-	4/8/8/8	0/3/3/3
2	EQ2	C	501	-	-	4/8/8/8	0/3/3/3
3	AMP	E	502	-	-	0/2/22/26	0/3/3/3
2	EQ2	B	501	-	-	8/8/8/8	0/3/3/3
2	EQ2	D	501	-	-	4/8/8/8	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	AMP	O4'-C1'	3.59	1.45	1.40
2	E	501	EQ2	C3-N1	3.55	1.35	1.32
2	E	501	EQ2	C6-C4	3.36	1.40	1.37
3	B	502	AMP	O4'-C1'	3.09	1.45	1.40
3	D	502	AMP	C2-N3	2.82	1.36	1.32
3	C	502	AMP	C2-N3	2.74	1.36	1.32
3	B	502	AMP	C2-N3	2.67	1.36	1.32
2	B	501	EQ2	C3-N1	2.66	1.34	1.32
3	E	502	AMP	C2-N3	2.57	1.36	1.32
3	D	502	AMP	O4'-C1'	2.50	1.44	1.40
3	A	502	AMP	O4'-C1'	2.50	1.44	1.40
3	A	502	AMP	C2-N3	2.31	1.35	1.32
2	A	501	EQ2	C3-N1	2.19	1.34	1.32
2	E	501	EQ2	C4-C5	2.09	1.54	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	EQ2	C6-C4	2.05	1.39	1.37
2	D	501	EQ2	C6-C4	2.02	1.39	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	AMP	N3-C2-N1	-4.94	121.97	128.67
3	D	502	AMP	N3-C2-N1	-4.78	122.19	128.67
3	B	502	AMP	O4'-C1'-N9	4.24	114.37	108.75
3	B	502	AMP	N3-C2-N1	-4.22	122.94	128.67
3	E	502	AMP	O4'-C1'-N9	4.18	114.28	108.75
3	E	502	AMP	N3-C2-N1	-3.77	123.56	128.67
3	A	502	AMP	N3-C2-N1	-3.08	124.49	128.67
3	A	502	AMP	C4'-O4'-C1'	2.99	112.66	109.92
2	A	501	EQ2	O3-C5-C4	-2.82	115.62	121.30
3	B	502	AMP	O4'-C4'-C5'	2.79	118.26	109.33
3	A	502	AMP	O4'-C1'-N9	2.58	112.16	108.75
3	D	502	AMP	C4'-O4'-C1'	2.50	112.22	109.92
3	A	502	AMP	C4-C5-N7	-2.50	106.69	109.34
3	A	502	AMP	C2'-C3'-C4'	2.46	107.36	102.61
3	A	502	AMP	C1'-N9-C4	-2.45	122.34	126.64
3	D	502	AMP	N6-C6-N1	2.36	123.37	118.33
3	B	502	AMP	O4'-C4'-C3'	-2.33	100.53	105.15
3	E	502	AMP	O4'-C4'-C5'	2.30	114.08	109.22
3	B	502	AMP	O5'-C5'-C4'	2.25	116.65	108.99
3	B	502	AMP	C2'-C3'-C4'	2.22	106.91	102.61
2	B	501	EQ2	O3-C5-C4	-2.19	116.89	121.30
2	D	501	EQ2	O3-C5-C4	-2.15	116.96	121.30
3	C	502	AMP	C1'-N9-C4	-2.11	122.93	126.64
3	C	502	AMP	O4'-C1'-N9	2.11	111.54	108.75
2	C	501	EQ2	C11-C12-C13	-2.10	117.22	120.09
2	D	501	EQ2	C11-C12-C13	-2.10	117.22	120.09
2	E	501	EQ2	C11-C12-C13	-2.10	117.22	120.09
2	A	501	EQ2	C11-C12-C13	-2.09	117.23	120.09
2	C	501	EQ2	O3-C5-C4	-2.05	117.18	121.30
3	A	502	AMP	O3'-C3'-C4'	-2.04	105.22	111.08
3	C	502	AMP	O2P-P-O1P	2.01	118.69	110.83
2	B	501	EQ2	C11-C12-C13	-2.00	117.35	120.09

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	EQ2	C1-C2-C3-C14
2	A	501	EQ2	O1-C2-C3-N1
2	A	501	EQ2	O1-C2-C3-C14
2	B	501	EQ2	C1-C2-C3-C14
2	B	501	EQ2	O1-C2-C3-C14
2	C	501	EQ2	C1-C2-C3-N1
2	C	501	EQ2	C1-C2-C3-C14
2	C	501	EQ2	O1-C2-C3-N1
2	C	501	EQ2	O1-C2-C3-C14
2	D	501	EQ2	C1-C2-C3-C14
2	D	501	EQ2	O1-C2-C3-N1
2	D	501	EQ2	O1-C2-C3-C14
2	E	501	EQ2	C1-C2-C3-N1
2	E	501	EQ2	C1-C2-C3-C14
2	E	501	EQ2	O1-C2-C3-N1
2	E	501	EQ2	O1-C2-C3-C14
3	B	502	AMP	O4'-C4'-C5'-O5'
3	B	502	AMP	C3'-C4'-C5'-O5'
2	B	501	EQ2	N1-C4-C5-O2
2	B	501	EQ2	N1-C4-C5-O3
2	B	501	EQ2	C6-C4-C5-O2
2	B	501	EQ2	O1-C2-C3-N1
2	D	501	EQ2	C1-C2-C3-N1
3	B	502	AMP	C5'-O5'-P-O1P
2	B	501	EQ2	C6-C4-C5-O3
2	A	501	EQ2	C1-C2-C3-N1
2	B	501	EQ2	C1-C2-C3-N1

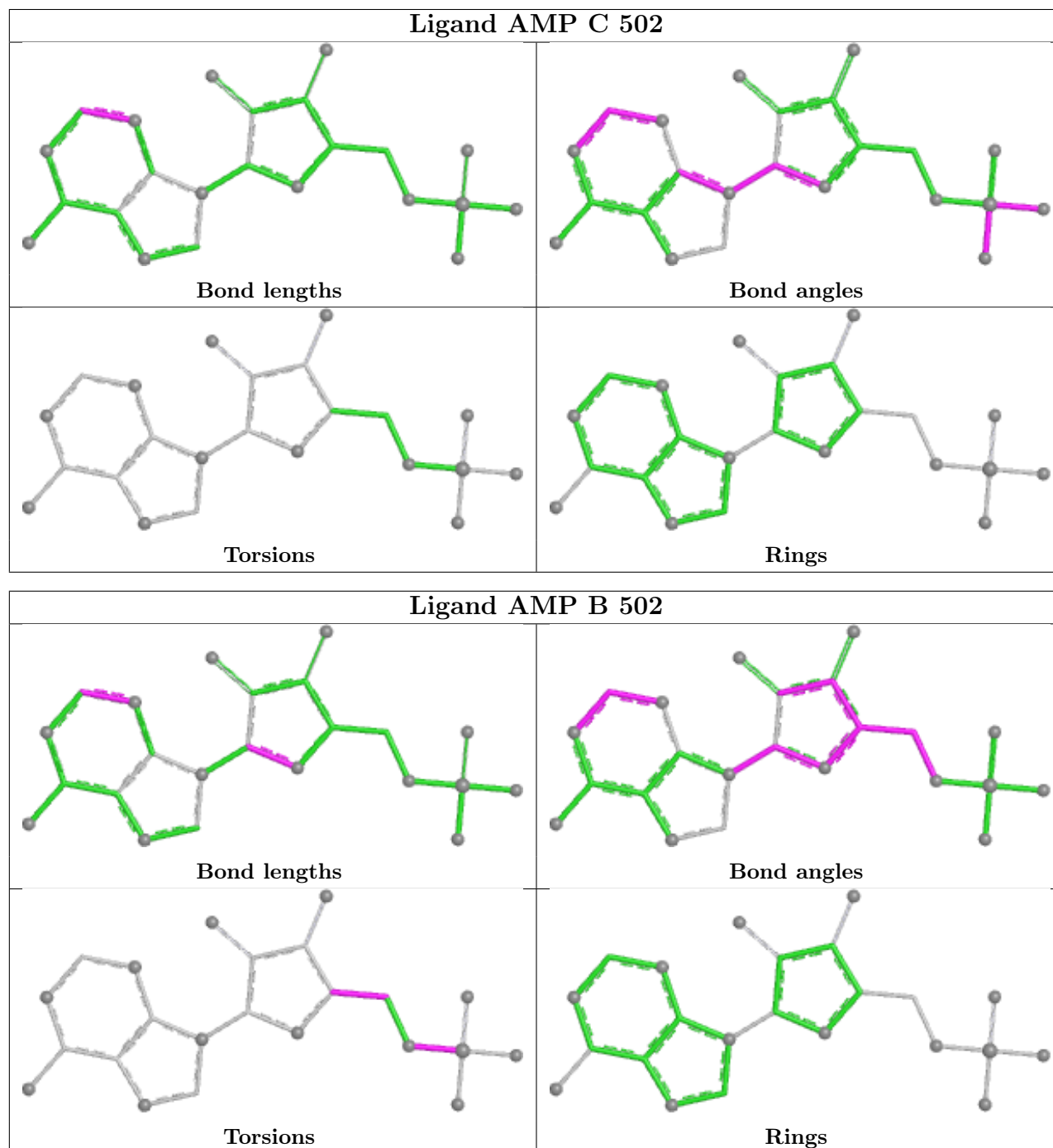
There are no ring outliers.

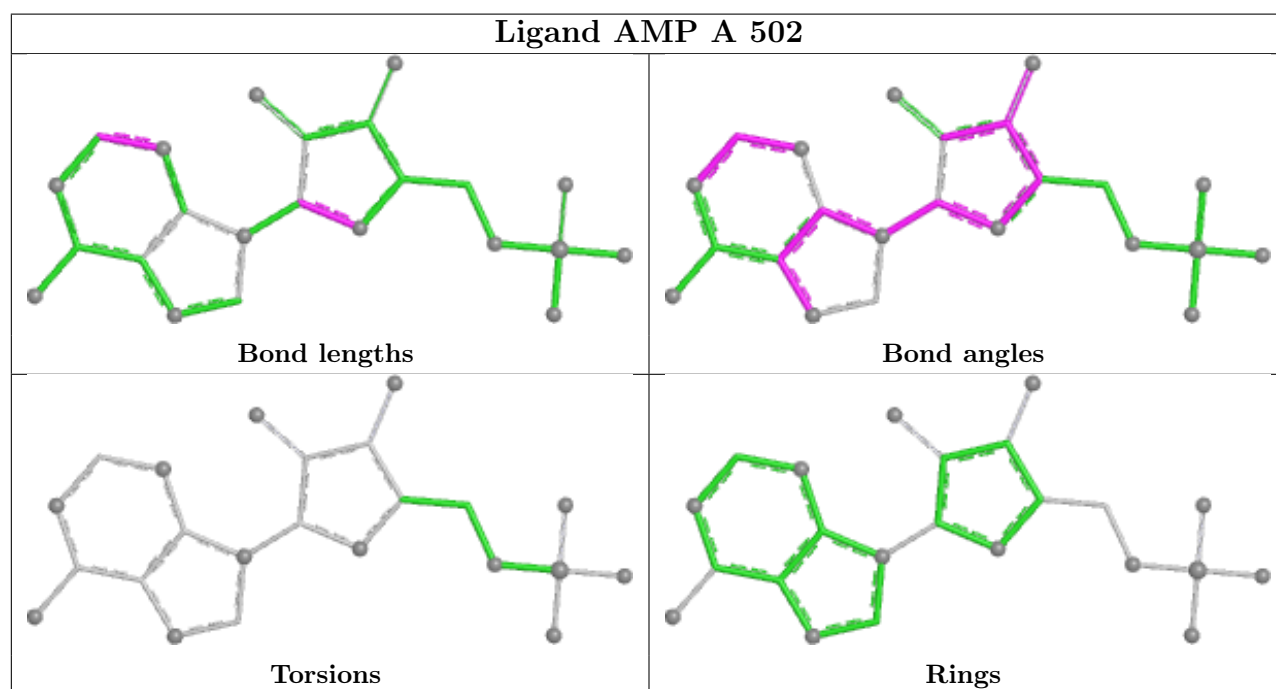
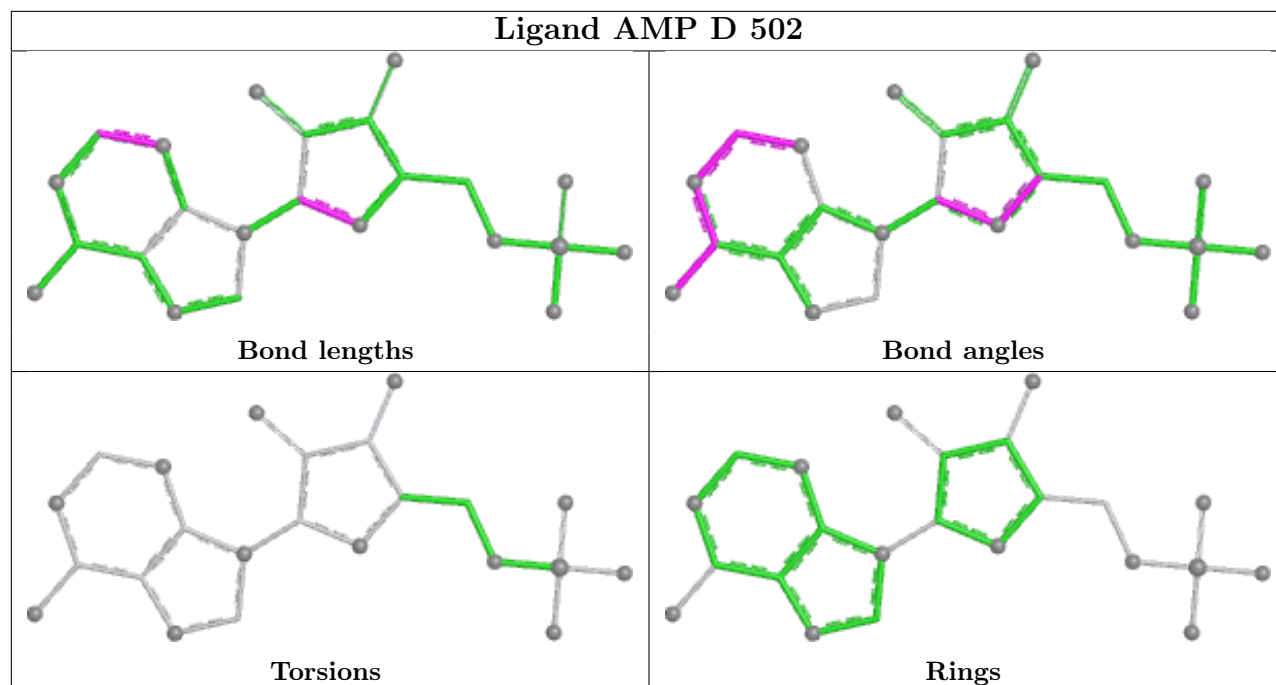
5 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	AMP	3	0
3	B	502	AMP	4	0
3	D	502	AMP	4	0
3	A	502	AMP	5	0
2	C	501	EQ2	2	0

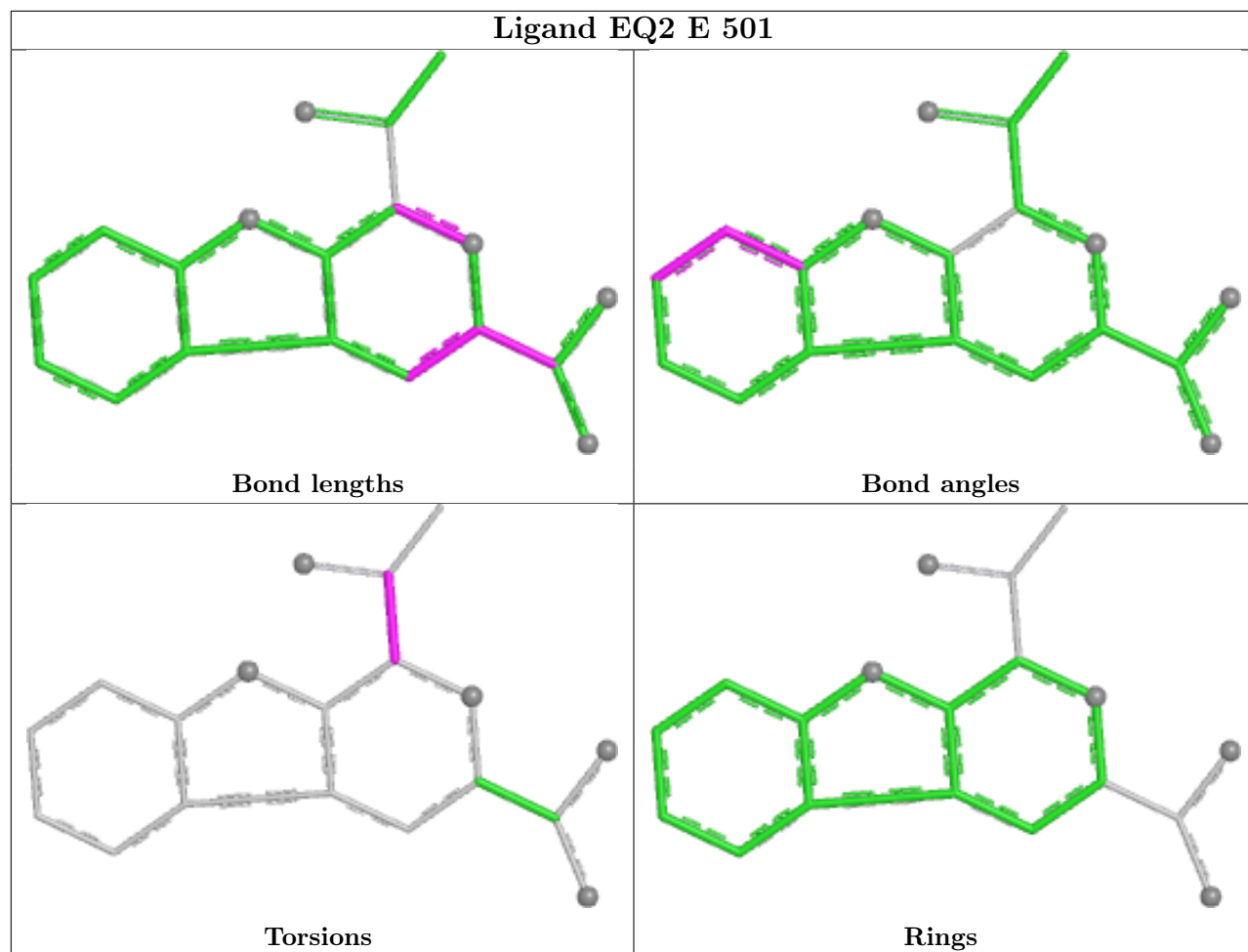
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

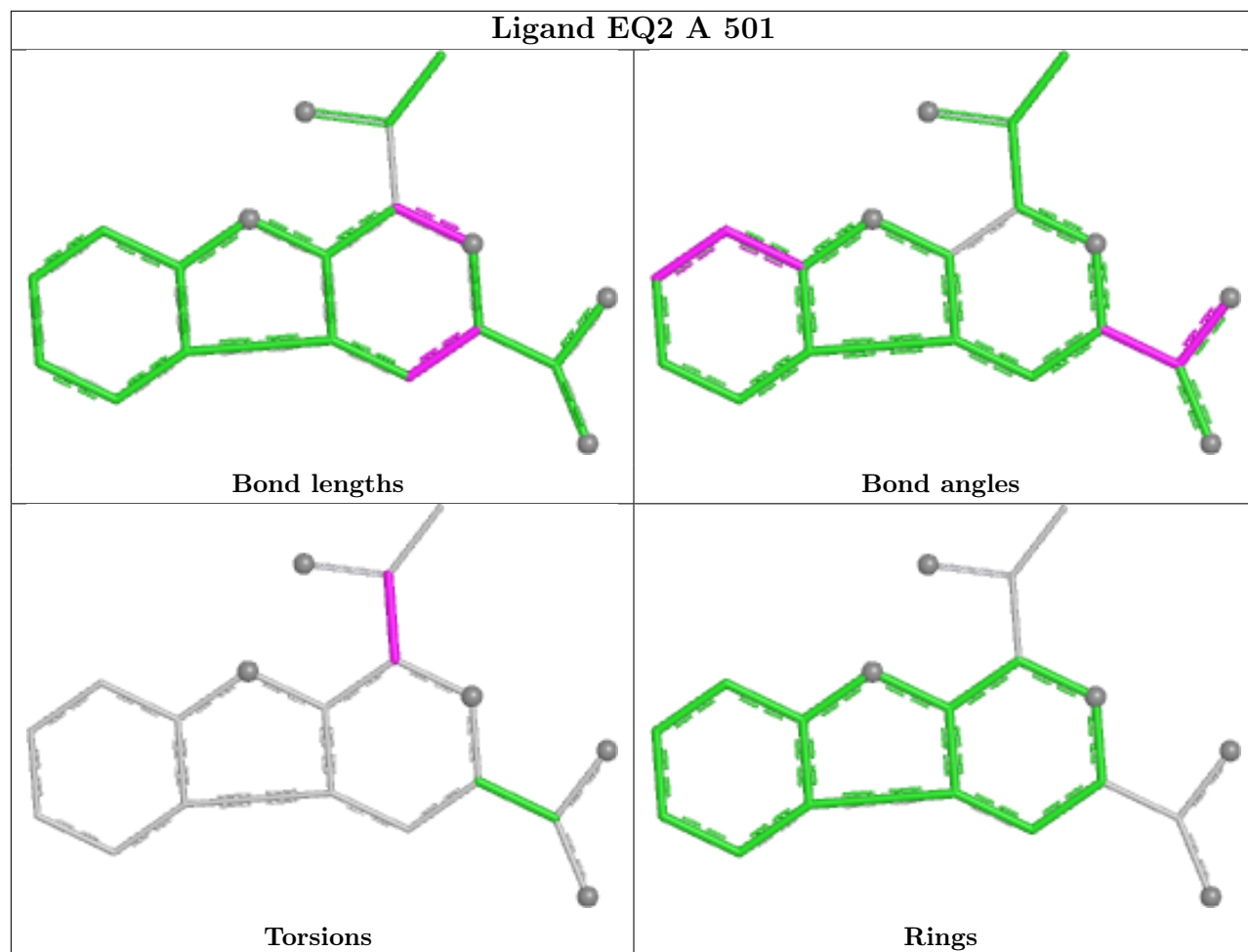




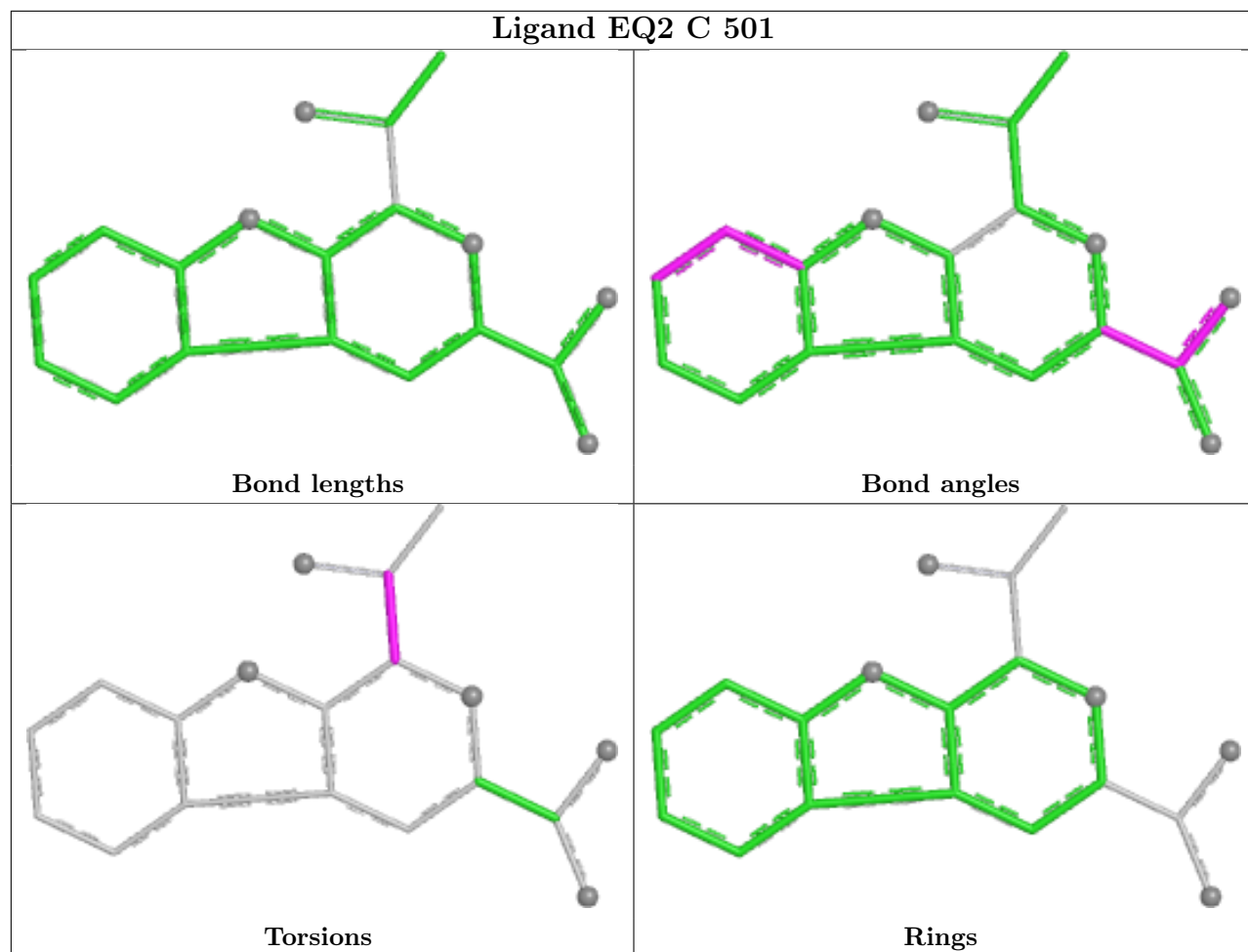
Ligand EQ2 E 501



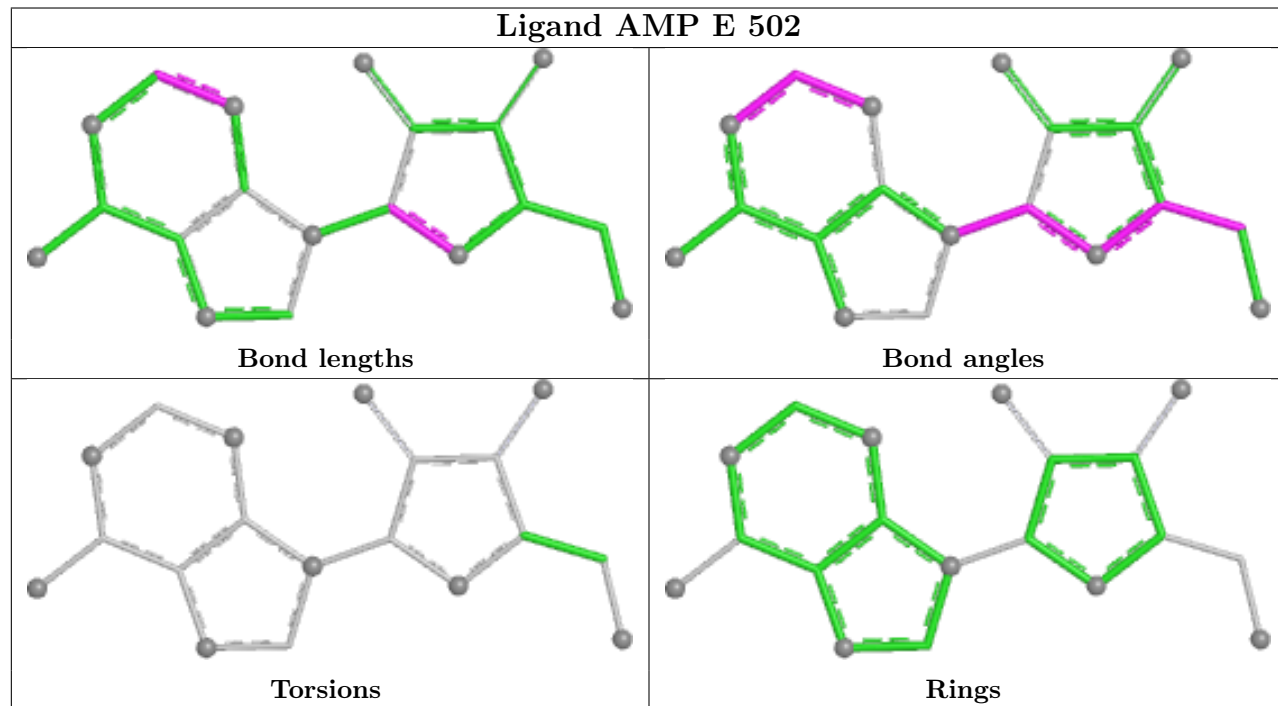
Ligand EQ2 A 501



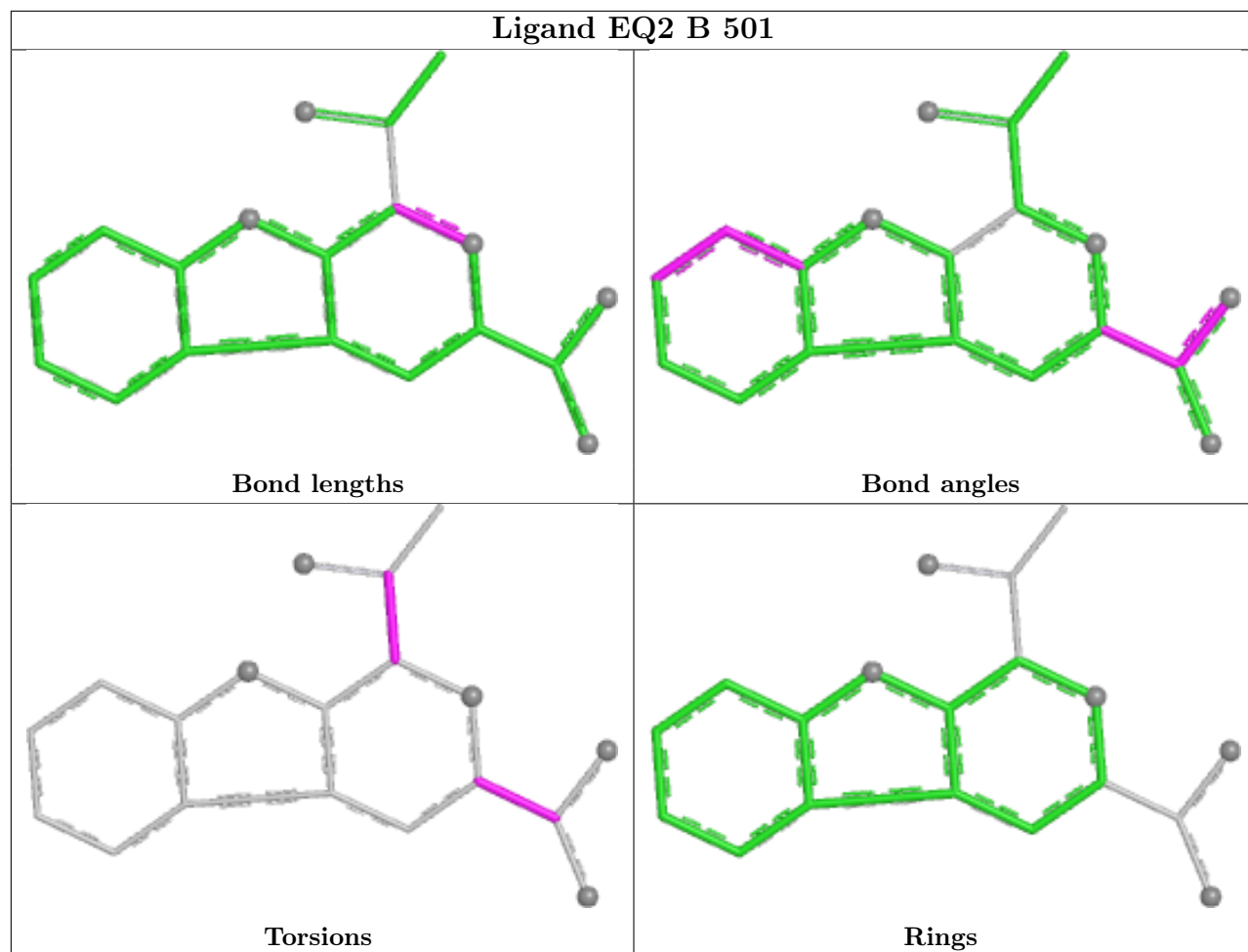
Ligand EQ2 C 501

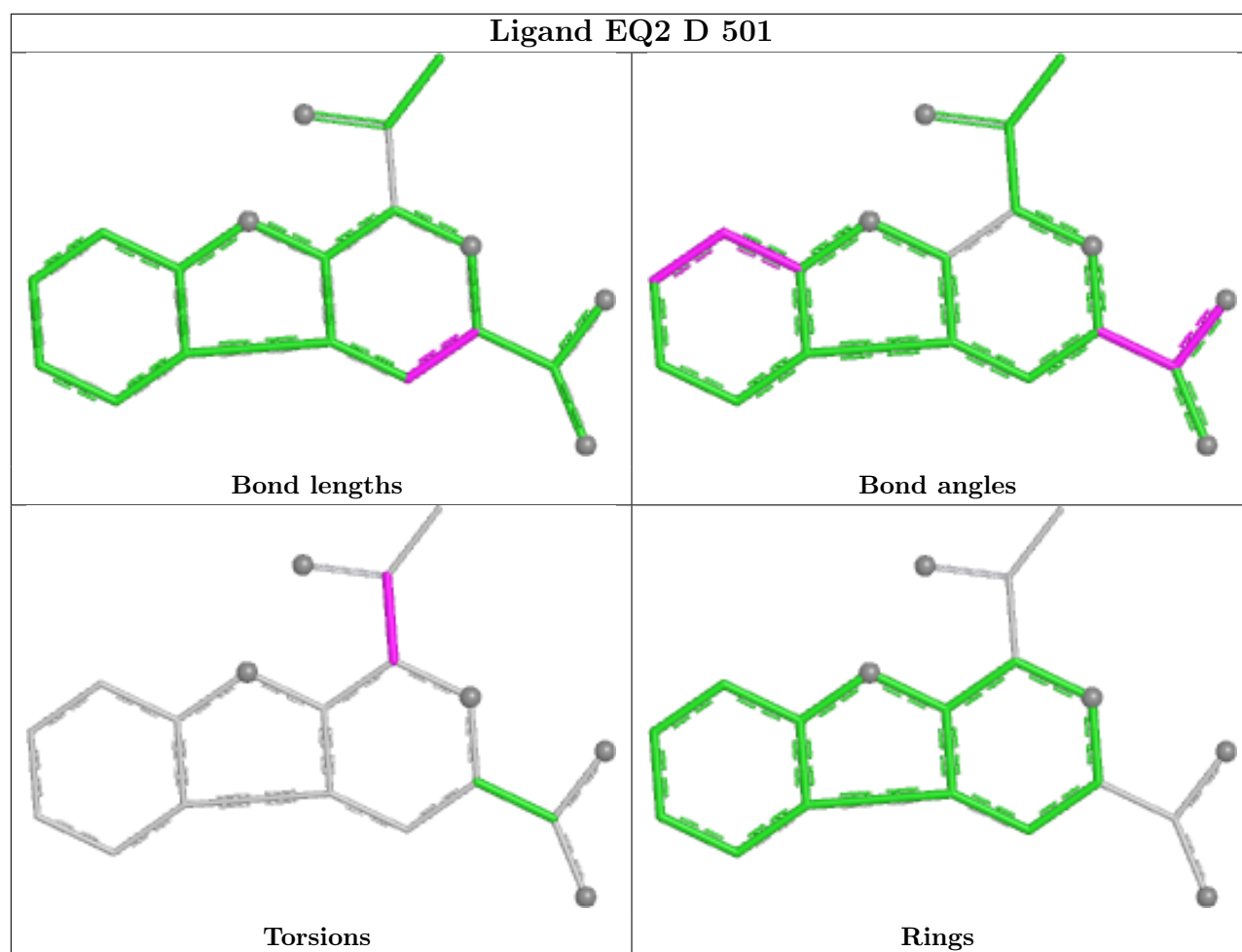


Ligand AMP E 502



Ligand EQ2 B 501





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	486/498 (97%)	0.10	10 (2%) 63 58	17, 36, 63, 95	0
1	B	494/498 (99%)	0.01	4 (0%) 86 84	19, 36, 64, 104	0
1	C	489/498 (98%)	-0.01	4 (0%) 86 84	19, 35, 63, 91	0
1	D	487/498 (97%)	0.09	8 (1%) 72 68	21, 37, 69, 90	0
1	E	494/498 (99%)	0.18	9 (1%) 68 64	27, 46, 77, 111	0
All	All	2450/2490 (98%)	0.07	35 (1%) 75 71	17, 39, 68, 111	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	PRO	4.4
1	E	19	ALA	3.8
1	A	432	SER	3.6
1	D	114	ARG	3.4
1	E	18	GLY	3.0
1	E	480	PRO	3.0
1	A	431	ASP	2.9
1	A	115	VAL	2.9
1	A	164	THR	2.9
1	D	116	SER	2.8
1	A	117	VAL	2.8
1	D	359	ARG	2.6
1	E	495	ASP	2.5
1	A	44	ILE	2.5
1	B	165	PRO	2.5
1	E	334	SER	2.4
1	B	115	VAL	2.4
1	D	108	ALA	2.4
1	E	339	PRO	2.3
1	D	98	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	98	LEU	2.3
1	B	89	ALA	2.3
1	E	259	SER	2.3
1	A	111	LEU	2.2
1	C	115	VAL	2.2
1	A	152	ILE	2.2
1	D	358	TRP	2.2
1	A	114	ARG	2.2
1	C	19	ALA	2.2
1	C	76	GLY	2.2
1	E	318	ALA	2.1
1	E	446	ALA	2.1
1	A	90	ILE	2.0
1	B	47	GLY	2.0
1	D	89	ALA	2.0

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 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.

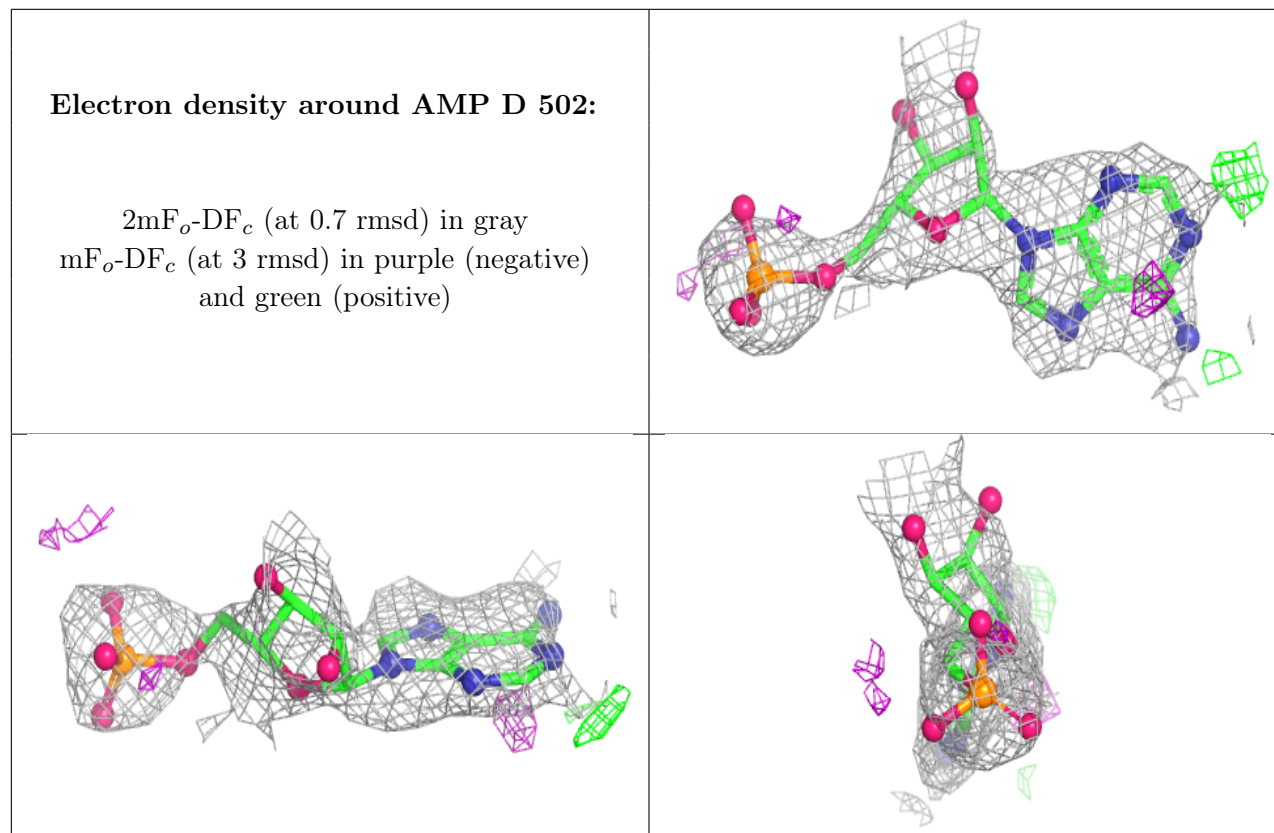
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	D	502	23/23	0.86	0.31	82,93,103,105	0
3	AMP	C	502	23/23	0.88	0.23	67,78,104,106	0
3	AMP	A	502	23/23	0.89	0.23	59,69,81,88	0
3	AMP	B	502	23/23	0.91	0.20	52,64,105,108	0
2	EQ2	E	501	19/19	0.94	0.16	41,55,61,63	0
3	AMP	E	502	19/23	0.94	0.20	47,52,55,55	0
2	EQ2	B	501	19/19	0.96	0.16	35,39,49,51	0
2	EQ2	D	501	19/19	0.96	0.19	36,38,43,43	0

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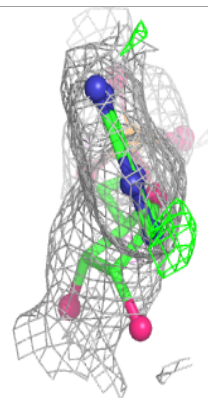
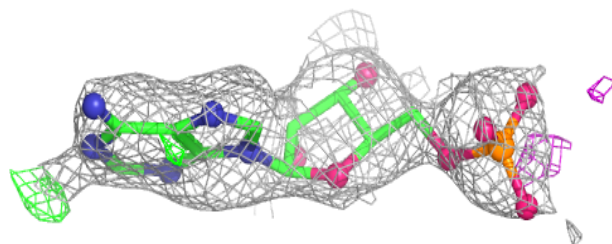
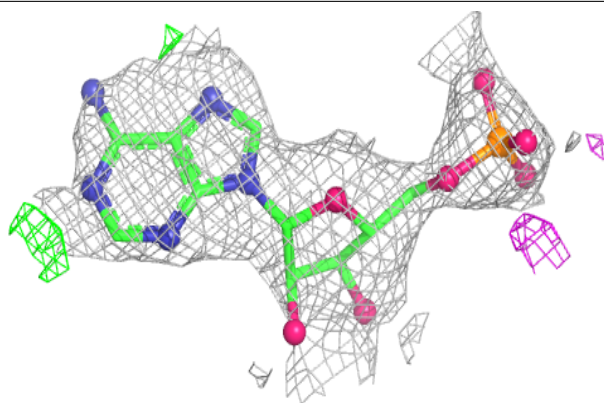
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EQ2	C	501	19/19	0.97	0.16	33,36,42,44	0
2	EQ2	A	501	19/19	0.97	0.15	34,37,45,45	0

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.

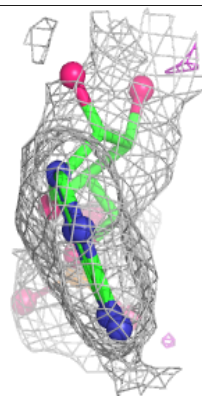
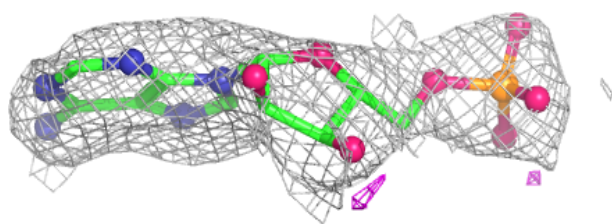
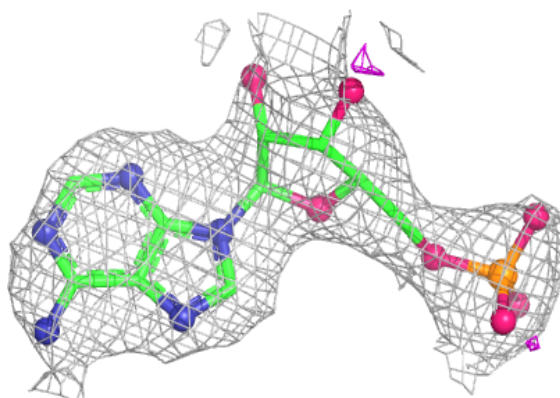


Electron density around AMP C 502:

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

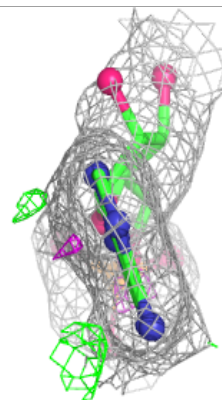
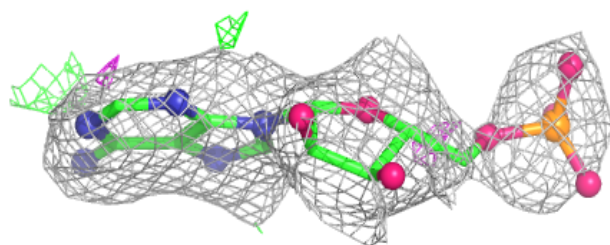
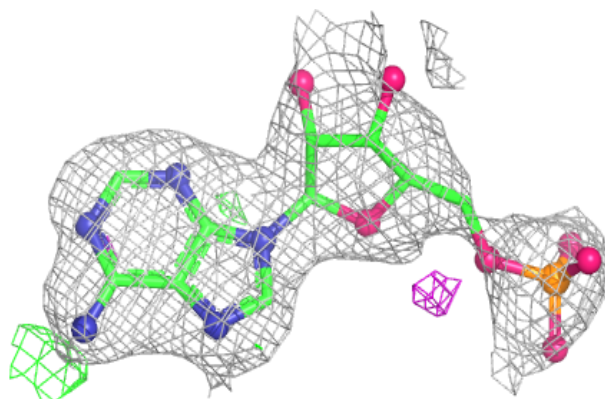
**Electron density around AMP A 502:**

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



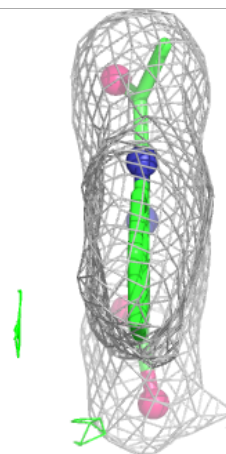
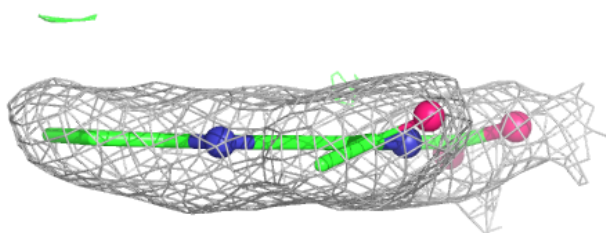
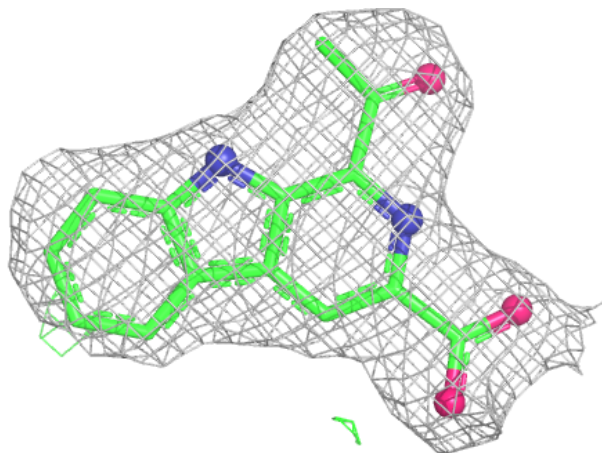
Electron density around AMP B 502:

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



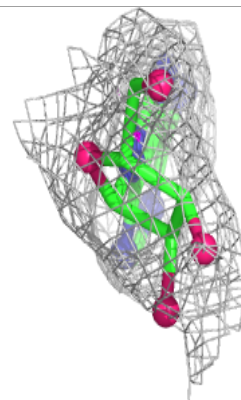
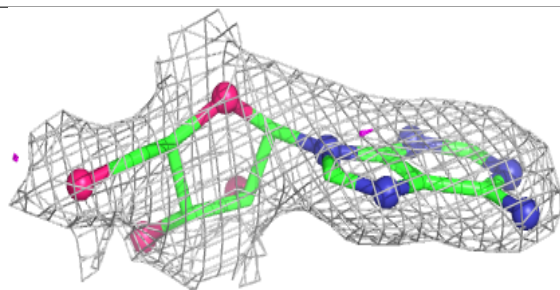
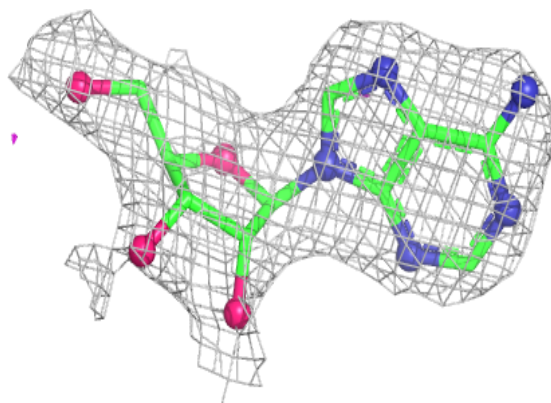
Electron density around EQ2 E 501:

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



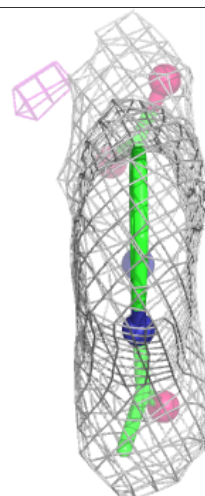
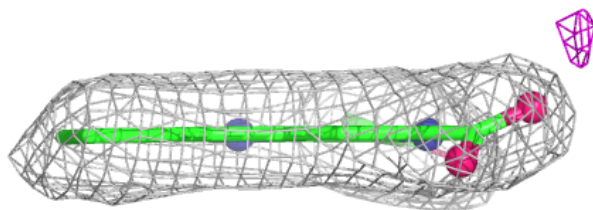
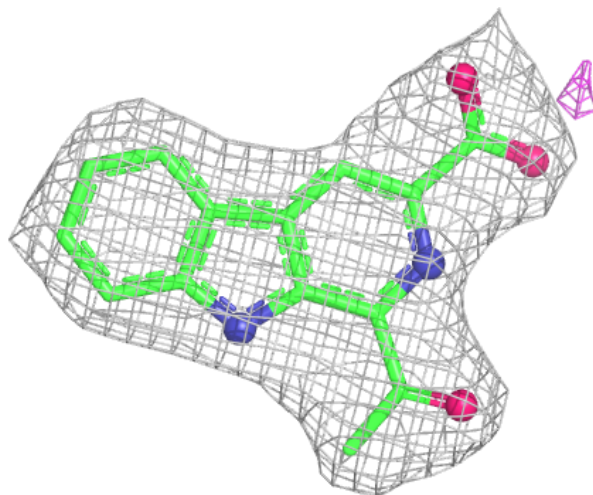
Electron density around AMP E 502:

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



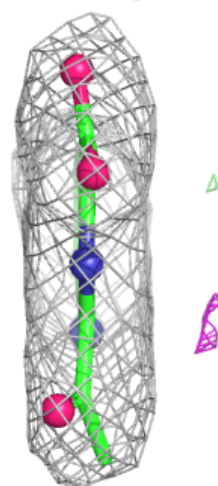
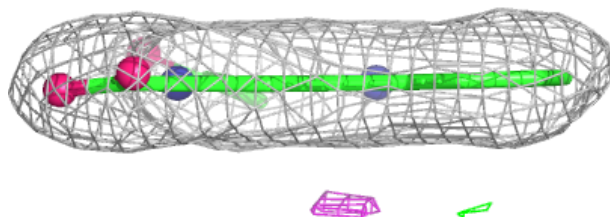
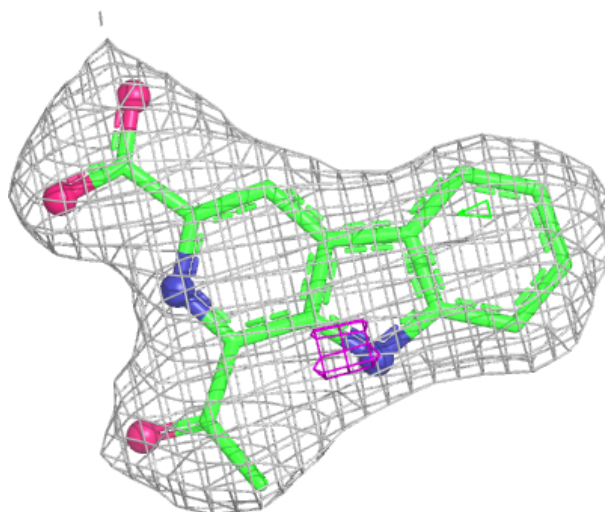
Electron density around EQ2 B 501:

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



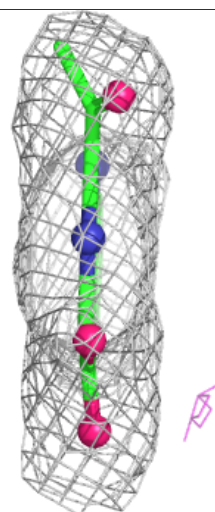
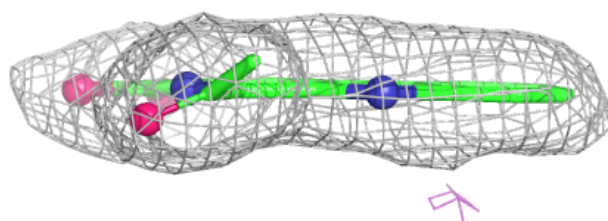
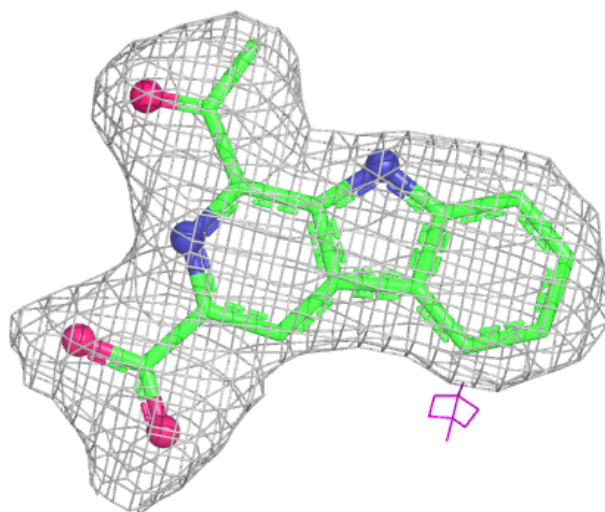
Electron density around EQ2 D 501:

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



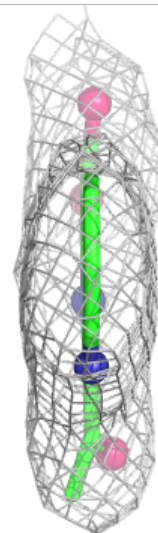
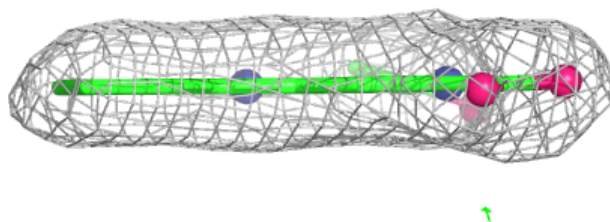
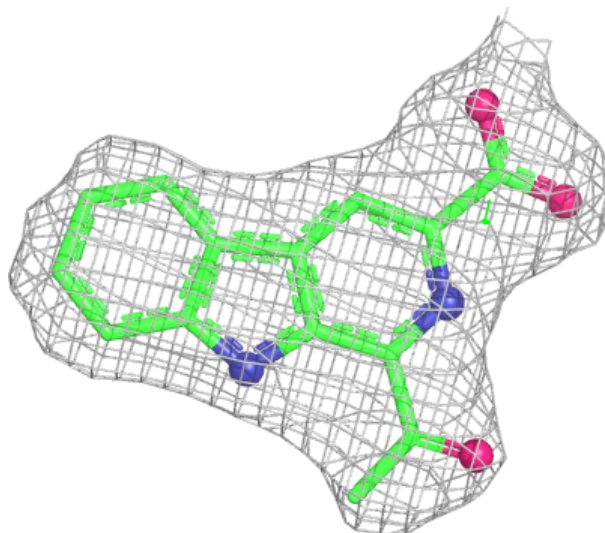
Electron density around EQ2 C 501:

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



Electron density around EQ2 A 501:

$2mF_o-DF_c$ (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.