



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 12:04 PM UTC

PDB ID : 6H1B / pdb_00006h1b
Title : Structure of amide bond synthetase Mcba K483A mutant from *Marinactinospora thermotolerans*
Authors : Rowlinson, B.; Petchey, M.; Cuetos, A.; Frese, A.; Dannevald, S.; Grogan, G.
Deposited on : 2018-07-11
Resolution : 2.80 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 : 4-5-2 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

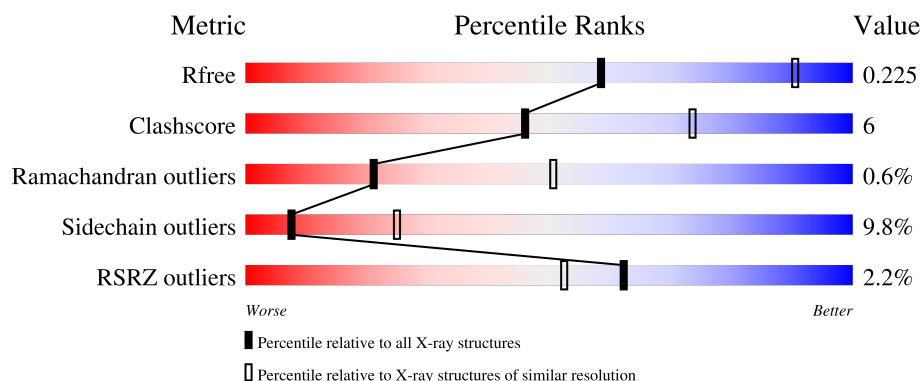
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	499	2% 81% 15% ..
1	B	499	2% 80% 14% ..
1	C	499	4% 84% 14% .
1	D	499	85% 12% .
1	E	499	3% 84% 13% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18101 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	487	Total	C	N	O	S	0	0	0
			3554	2253	639	649	13			
1	B	485	Total	C	N	O	S	0	0	0
			3534	2237	635	649	13			
1	C	490	Total	C	N	O	S	0	2	0
			3575	2257	651	654	13			
1	D	487	Total	C	N	O	S	0	0	0
			3536	2238	636	649	13			
1	E	487	Total	C	N	O	S	0	0	0
			3502	2225	628	637	12			

There are 25 discrepancies between the modelled and reference sequences:

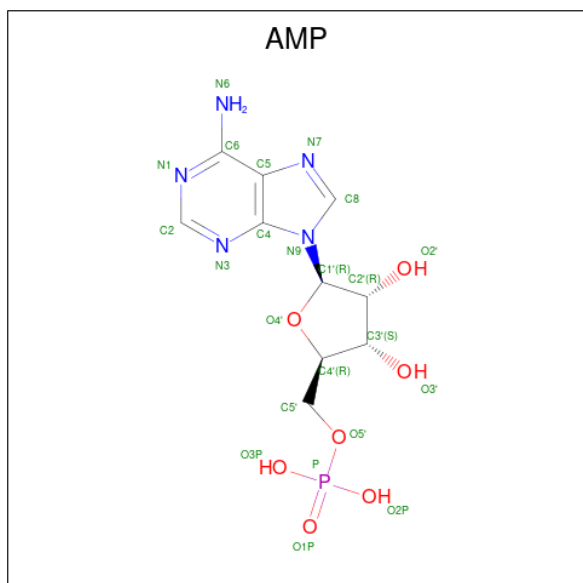
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLN	-	expression tag	UNP R4R1U5
A	-2	GLY	-	expression tag	UNP R4R1U5
A	-1	PRO	-	expression tag	UNP R4R1U5
A	0	ALA	-	expression tag	UNP R4R1U5
A	483	ALA	LYS	engineered mutation	UNP R4R1U5
B	-3	GLN	-	expression tag	UNP R4R1U5
B	-2	GLY	-	expression tag	UNP R4R1U5
B	-1	PRO	-	expression tag	UNP R4R1U5
B	0	ALA	-	expression tag	UNP R4R1U5
B	483	ALA	LYS	engineered mutation	UNP R4R1U5
C	-3	GLN	-	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
C	483	ALA	LYS	engineered mutation	UNP R4R1U5
D	-3	GLN	-	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

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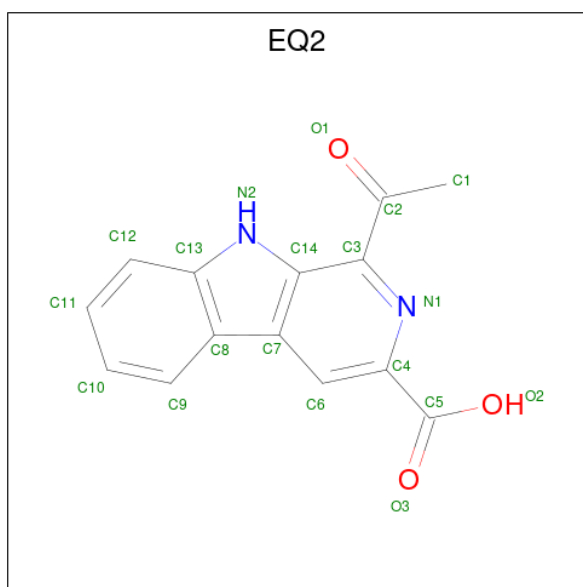
Chain	Residue	Modelled	Actual	Comment	Reference
D	483	ALA	LYS	engineered mutation	UNP R4R1U5
E	-3	GLN	-	expression tag	UNP R4R1U5
E	-2	GLY	-	expression tag	UNP R4R1U5
E	-1	PRO	-	expression tag	UNP R4R1U5
E	0	ALA	-	expression tag	UNP R4R1U5
E	483	ALA	LYS	engineered mutation	UNP R4R1U5

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is 1-ethanoyl-9 {H}-pyrido[3,4-b]indole-3-carboxylic acid (CCD ID: EQ2) (formula: $C_{14}H_{10}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



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

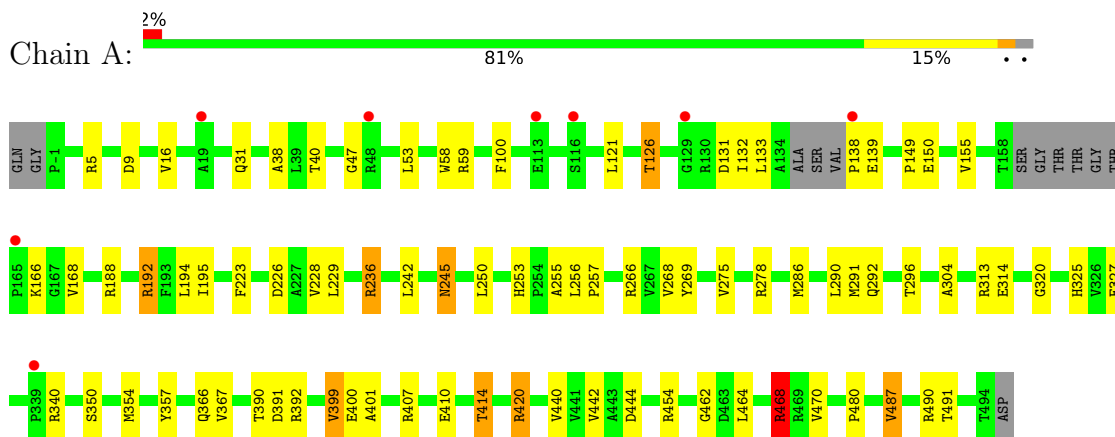
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	44	Total	O	0	0
			44	44		
4	C	49	Total	O	0	0
			49	49		
4	D	29	Total	O	0	0
			29	29		
4	E	26	Total	O	0	0
			26	26		

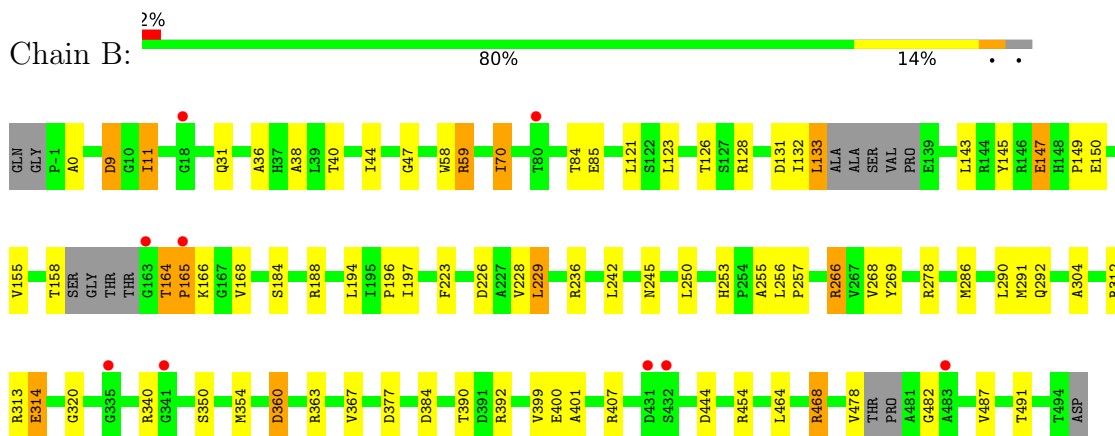
3 Residue-property plots [i](#)

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.

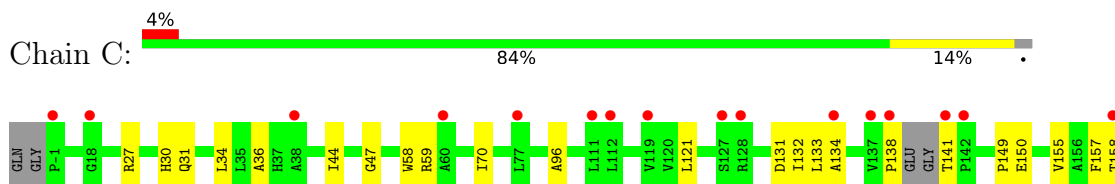
• Molecule 1: Fatty acid CoA ligase

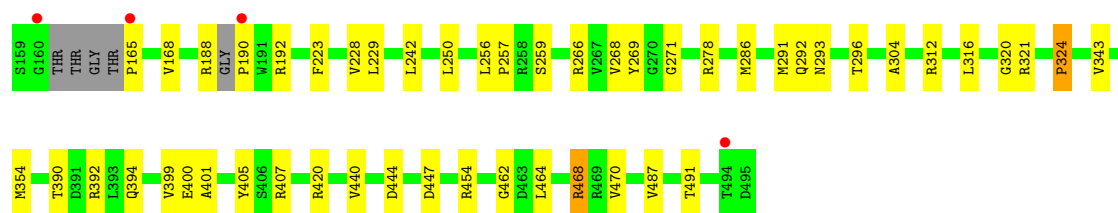


• Molecule 1: Fatty acid CoA ligase



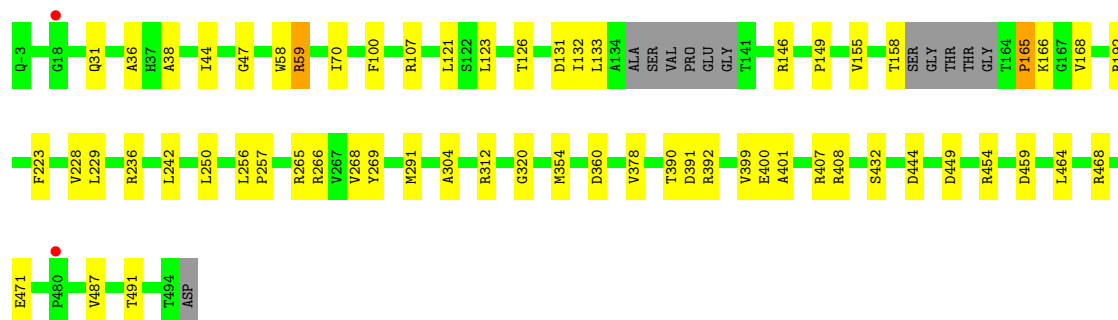
• Molecule 1: Fatty acid CoA ligase





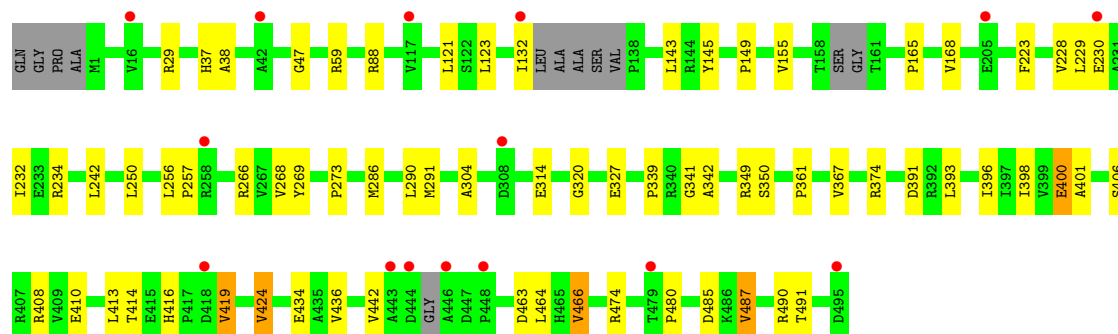
● Molecule 1: Fatty acid CoA ligase

Chain D: 85% 12% .



● Molecule 1: Fatty acid CoA ligase

Chain E: 3% 84% 13% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.23Å 130.74Å 196.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	101.50 – 2.80 101.50 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (101.50-2.80) 79.8 (101.50-2.80)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.204 , 0.248 (Not available) , 0.225	Depositor DCC
R_{free} test set	3618 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtriage
Anisotropy	0.523	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18101	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: 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	0.89	4/3636 (0.1%)	1.07	1/4980 (0.0%)
1	B	0.88	0/3612	1.09	4/4945 (0.1%)
1	C	0.88	3/3661 (0.1%)	1.08	4/5008 (0.1%)
1	D	0.88	0/3617	1.07	1/4959 (0.0%)
1	E	0.87	1/3581 (0.0%)	1.08	0/4909
All	All	0.88	8/18107 (0.0%)	1.08	10/24801 (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	4
1	B	0	3
1	C	0	6
1	D	0	4
1	E	0	6
All	All	0	23

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	470	VAL	C-O	-6.91	1.16	1.24
1	C	316	LEU	C-O	-6.03	1.16	1.24
1	E	396	ILE	C-O	-5.87	1.18	1.24
1	A	16	VAL	C-O	-5.55	1.18	1.24
1	C	470	VAL	C-O	-5.33	1.18	1.24
1	C	440	VAL	C-O	-5.30	1.18	1.24
1	A	440	VAL	C-O	-5.10	1.18	1.24
1	A	462	GLY	C-O	-5.09	1.18	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	360	ASP	CA-CB-CG	9.16	121.76	112.60
1	D	360	ASP	CA-CB-CG	8.95	121.55	112.60
1	A	462	GLY	CA-C-O	-7.38	116.11	122.16
1	B	11	ILE	CA-C-O	-6.40	112.78	120.78
1	B	11	ILE	CB-CA-C	5.21	119.83	111.29
1	C	157	PHE	CA-C-N	5.17	130.79	121.06
1	C	157	PHE	C-N-CA	5.17	130.79	121.06
1	B	9	ASP	CA-CB-CG	5.13	117.73	112.60
1	C	286	MET	CA-C-N	-5.08	115.99	122.19
1	C	286	MET	C-N-CA	-5.08	115.99	122.19

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	340	ARG	Sidechain
1	A	420	ARG	Sidechain
1	A	468	ARG	Sidechain
1	A	59	ARG	Sidechain
1	B	266	ARG	Sidechain
1	B	468	ARG	Sidechain
1	B	59	ARG	Sidechain
1	C	266	ARG	Sidechain
1	C	27	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	321	ARG	Sidechain
1	C	468	ARG	Sidechain
1	C	59	ARG	Sidechain
1	D	107	ARG	Sidechain
1	D	146	ARG	Sidechain
1	D	408	ARG	Sidechain
1	D	59	ARG	Sidechain
1	E	266	ARG	Sidechain
1	E	29	ARG	Sidechain
1	E	374	ARG	Sidechain
1	E	408	ARG	Sidechain
1	E	474	ARG	Sidechain
1	E	88	ARG	Sidechain

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	3554	0	3484	46	0
1	B	3534	0	3465	41	0
1	C	3575	0	3473	51	0
1	D	3536	0	3443	39	0
1	E	3502	0	3395	36	0
2	A	23	0	12	1	0
2	B	23	0	12	2	0
2	C	23	0	12	2	0
2	D	23	0	12	1	0
2	E	19	0	12	1	0
3	A	19	0	0	0	0
3	B	19	0	0	0	0
3	C	19	0	0	1	0
3	D	19	0	0	0	0
3	E	19	0	0	0	0
4	A	46	0	0	3	0
4	B	44	0	0	4	0
4	C	49	0	0	7	0
4	D	29	0	0	0	0
4	E	26	0	0	1	0
All	All	18101	0	17320	204	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 6.

All (204) 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:E:410:GLU:HG3	1:E:424:VAL:HG13	1.39	1.03
1:C:192:ARG:HH11	1:C:192:ARG:HG2	1.27	0.95
1:D:392:ARG:NH1	2:D:501:AMP:O3'	2.05	0.89
1:C:138:PRO:C	1:C:141:THR:N	2.31	0.88
1:C:392:ARG:NH1	2:C:501:AMP:O3'	2.11	0.83
1:C:138:PRO:O	1:C:141:THR:N	2.12	0.82
1:A:392:ARG:NH1	2:A:501:AMP:O3'	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:VAL:HG13	1:A:354:MET:HE3	1.62	0.82
1:C:192:ARG:HG2	1:C:192:ARG:NH1	1.94	0.81
1:D:168:VAL:HG13	1:D:354:MET:HE3	1.62	0.81
1:C:36:ALA:O	1:C:70:ILE:HD11	1.80	0.80
1:C:168:VAL:HG13	1:C:354:MET:HE3	1.65	0.79
1:A:327:GLU:OE1	1:B:340:ARG:CB	2.31	0.78
1:E:410:GLU:CG	1:E:424:VAL:HG13	2.14	0.78
1:D:36:ALA:O	1:D:70:ILE:HD11	1.83	0.78
1:B:392:ARG:NH1	2:B:501:AMP:O3'	2.17	0.77
1:B:168:VAL:HG13	1:B:354:MET:HE3	1.65	0.77
1:D:378:VAL:HG12	1:D:391:ASP:O	1.85	0.76
1:D:192:ARG:NH1	1:D:236:ARG:O	2.18	0.76
1:A:192:ARG:HG2	1:A:192:ARG:HH11	1.49	0.76
1:A:192:ARG:NH1	1:A:236:ARG:O	2.22	0.72
1:C:30:HIS:CD2	4:C:616:HOH:O	2.42	0.71
1:C:30:HIS:HD2	4:C:616:HOH:O	1.74	0.71
1:C:34:LEU:HD12	1:C:34:LEU:C	2.18	0.69
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.05	0.69
1:C:394:GLN:HG3	4:C:624:HOH:O	1.94	0.68
1:A:245:ASN:ND2	4:A:602:HOH:O	2.28	0.66
1:E:463:ASP:O	1:E:466:VAL:CG1	2.43	0.66
1:A:31:GLN:HE22	1:A:133:LEU:CD2	2.09	0.65
1:A:5:ARG:HH11	1:D:432:SER:HB3	1.62	0.65
1:E:463:ASP:O	1:E:466:VAL:HG12	1.97	0.64
1:D:31:GLN:HE22	1:D:133:LEU:CD2	2.12	0.62
1:E:143:LEU:C	1:E:143:LEU:HD23	2.25	0.62
1:B:229:LEU:HD13	1:B:250:LEU:HD11	1.82	0.61
1:A:192:ARG:HH12	1:A:236:ARG:C	2.08	0.60
1:E:485:ASP:CB	4:E:601:HOH:O	2.48	0.60
1:D:229:LEU:HD13	1:D:250:LEU:HD11	1.83	0.60
1:E:410:GLU:HG3	1:E:424:VAL:CG1	2.25	0.60
1:C:271:GLY:O	4:C:602:HOH:O	2.17	0.59
1:D:454:ARG:NH1	1:D:468:ARG:O	2.36	0.59
1:A:454:ARG:NH1	1:A:468:ARG:O	2.36	0.59
1:B:454:ARG:NH1	1:B:468:ARG:O	2.36	0.59
1:C:454:ARG:NH1	1:C:468:ARG:O	2.36	0.58
1:D:256:LEU:HB3	1:D:257:PRO:HD3	1.86	0.57
1:A:229:LEU:HD13	1:A:250:LEU:HD11	1.86	0.57
1:D:31:GLN:HE22	1:D:133:LEU:HD21	1.69	0.57
1:B:399:VAL:HG21	1:B:464:LEU:HD22	1.86	0.57
1:C:259:SER:O	4:C:601:HOH:O	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:ILE:CG2	1:C:70:ILE:O	2.54	0.55
1:C:229:LEU:HD13	1:C:250:LEU:HD11	1.90	0.54
1:E:242:LEU:O	1:E:269:TYR:HA	2.07	0.54
1:E:256:LEU:HB3	1:E:257:PRO:HD3	1.88	0.54
1:B:242:LEU:O	1:B:269:TYR:HA	2.08	0.54
1:D:242:LEU:O	1:D:269:TYR:HA	2.08	0.53
1:C:132:ILE:C	1:C:134:ALA:H	2.16	0.53
1:C:242:LEU:O	1:C:269:TYR:HA	2.08	0.53
1:A:410:GLU:O	1:A:414:THR:HB	2.09	0.53
1:A:31:GLN:HE22	1:A:133:LEU:HD21	1.72	0.53
1:A:188:ARG:NH2	1:D:449:ASP:OD2	2.42	0.53
1:A:242:LEU:O	1:A:269:TYR:HA	2.09	0.53
1:A:275:VAL:HG13	1:A:414:THR:HG21	1.90	0.53
1:C:188:ARG:O	1:C:190:PRO:N	2.42	0.53
1:A:400:GLU:O	1:A:401:ALA:HB3	2.09	0.53
1:C:400:GLU:O	1:C:401:ALA:HB3	2.09	0.53
1:D:399:VAL:HG21	1:D:464:LEU:HD22	1.91	0.52
1:B:400:GLU:O	1:B:401:ALA:HB3	2.09	0.52
1:C:192:ARG:HH11	1:C:192:ARG:CG	2.07	0.52
1:E:416:HIS:HB3	1:E:419:VAL:HG13	1.92	0.52
1:A:138:PRO:HA	1:A:139:GLU:OE2	2.10	0.52
1:E:229:LEU:HD13	1:E:250:LEU:HD11	1.91	0.51
1:A:192:ARG:NH1	1:A:192:ARG:CG	2.71	0.51
1:C:399:VAL:HG21	1:C:464:LEU:HD22	1.93	0.50
1:D:70:ILE:O	1:D:70:ILE:CG2	2.59	0.50
1:B:31:GLN:HG3	1:B:58:TRP:CH2	2.46	0.50
1:E:398:ILE:O	1:E:434:GLU:HB2	2.12	0.49
1:D:400:GLU:O	1:D:401:ALA:HB3	2.12	0.49
1:B:131:ASP:OD1	1:B:133:LEU:N	2.46	0.49
1:B:487:VAL:O	1:B:491:THR:HG23	2.13	0.49
1:A:268:VAL:HA	1:A:291:MET:O	2.13	0.49
1:A:399:VAL:HG21	1:A:464:LEU:HD22	1.92	0.49
1:C:31:GLN:HG3	1:C:58:TRP:CH2	2.48	0.49
1:C:462:GLY:HA3	4:C:631:HOH:O	2.12	0.49
1:E:487:VAL:O	1:E:491:THR:HG23	2.13	0.49
1:C:487:VAL:O	1:C:491:THR:HG23	2.14	0.48
1:C:268:VAL:HA	1:C:291:MET:O	2.13	0.48
1:E:463:ASP:O	1:E:466:VAL:HG13	2.13	0.48
1:A:325:HIS:ND1	1:B:384:ASP:OD1	2.47	0.48
1:D:31:GLN:HG3	1:D:58:TRP:CH2	2.48	0.48
1:A:487:VAL:O	1:A:491:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ALA:CB	1:B:132:ILE:HG23	2.43	0.48
1:E:268:VAL:HA	1:E:291:MET:O	2.13	0.48
1:B:70:ILE:CG2	1:B:70:ILE:O	2.61	0.48
1:B:223:PHE:CD1	1:B:228:VAL:HG21	2.49	0.48
1:D:38:ALA:CB	1:D:132:ILE:HG23	2.44	0.48
1:D:487:VAL:O	1:D:491:THR:HG23	2.13	0.48
1:B:268:VAL:HA	1:B:291:MET:O	2.14	0.48
1:C:70:ILE:O	1:C:70:ILE:HG23	2.12	0.48
1:A:131:ASP:OD1	1:A:133:LEU:N	2.47	0.48
1:D:268:VAL:HA	1:D:291:MET:O	2.12	0.47
1:B:36:ALA:HB1	1:B:70:ILE:HD11	1.95	0.47
1:D:158:THR:HG22	1:D:165:PRO:O	2.14	0.47
1:E:400:GLU:O	1:E:401:ALA:HB3	2.14	0.47
1:B:36:ALA:HB1	1:B:70:ILE:CD1	2.45	0.47
1:C:343:VAL:HG11	1:C:405:TYR:OH	2.14	0.47
1:D:471:GLU:HG2	1:E:361:PRO:HG3	1.96	0.47
1:A:31:GLN:HG3	1:A:58:TRP:CH2	2.50	0.47
1:C:34:LEU:HD12	1:C:34:LEU:O	2.14	0.47
1:D:131:ASP:OD1	1:D:133:LEU:N	2.46	0.47
1:E:273:PRO:HA	2:E:501:AMP:C2	2.49	0.47
1:A:313:ARG:NH2	4:A:604:HOH:O	2.43	0.47
1:E:327:GLU:OE2	1:E:349:ARG:HD2	2.15	0.47
1:E:59:ARG:HB3	1:E:123:LEU:HD23	1.97	0.47
1:E:132:ILE:O	1:E:132:ILE:HG22	2.13	0.47
1:E:223:PHE:CD1	1:E:228:VAL:HG21	2.50	0.46
1:A:38:ALA:CB	1:A:132:ILE:HG23	2.45	0.46
1:E:416:HIS:HB3	1:E:419:VAL:CG1	2.45	0.46
1:B:165:PRO:HD2	4:B:641:HOH:O	2.14	0.46
1:C:447:ASP:OD2	1:E:37:HIS:NE2	2.49	0.46
1:B:164:THR:HG22	4:B:641:HOH:O	2.16	0.46
1:B:399:VAL:O	1:B:399:VAL:CG2	2.64	0.46
1:C:131:ASP:OD1	1:C:133:LEU:N	2.48	0.46
1:E:406:SER:HB3	1:E:424:VAL:HG22	1.97	0.46
1:C:34:LEU:C	1:C:34:LEU:CD1	2.89	0.45
1:A:5:ARG:NH1	1:D:432:SER:HB3	2.28	0.45
1:D:70:ILE:O	1:D:70:ILE:HG23	2.16	0.45
1:D:266:ARG:HH11	1:D:266:ARG:HG3	1.81	0.45
1:A:121:LEU:HB3	1:A:132:ILE:HG13	1.99	0.45
1:E:143:LEU:HD22	1:E:145:TYR:CZ	2.52	0.45
1:D:121:LEU:HB3	1:D:132:ILE:HG13	1.99	0.44
1:C:296:THR:HA	2:C:501:AMP:H5'1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:ASN:HB3	3:C:502:EQ2:C1	2.47	0.44
1:B:478:VAL:CG2	1:B:482:GLY:HA2	2.48	0.44
1:B:314:GLU:HG2	4:B:640:HOH:O	2.17	0.44
1:B:0:ALA:HB3	1:B:147:GLU:HG3	1.99	0.44
1:D:223:PHE:CD1	1:D:228:VAL:HG21	2.53	0.44
1:E:121:LEU:HB3	1:E:132:ILE:HG13	1.99	0.44
1:C:256:LEU:N	1:C:257:PRO:HD2	2.33	0.43
1:A:399:VAL:O	1:A:399:VAL:CG2	2.67	0.43
1:A:275:VAL:HG13	1:A:414:THR:CG2	2.49	0.43
1:B:121:LEU:HB3	1:B:132:ILE:HG13	2.00	0.43
1:C:133:LEU:N	1:C:133:LEU:CD1	2.82	0.43
1:C:304:ALA:O	1:C:320:GLY:HA3	2.18	0.43
1:E:230:GLU:CB	1:E:234:ARG:NH1	2.81	0.43
1:C:121:LEU:HB3	1:C:132:ILE:HG13	2.00	0.43
1:B:47:GLY:HA2	1:B:149:PRO:HD2	2.01	0.43
1:C:155:VAL:HA	1:C:168:VAL:O	2.19	0.43
1:C:324:PRO:HB2	4:C:629:HOH:O	2.18	0.43
1:B:312:ARG:NH2	1:D:459:ASP:OD2	2.41	0.43
1:B:304:ALA:O	1:B:320:GLY:HA3	2.19	0.43
1:D:390:THR:O	1:D:407:ARG:HB2	2.19	0.43
1:D:265:ARG:O	1:D:266:ARG:NH1	2.52	0.42
1:E:339:PRO:O	1:E:341:GLY:O	2.38	0.42
1:B:377:ASP:OD2	2:B:501:AMP:O3'	2.35	0.42
1:B:390:THR:O	1:B:407:ARG:HB2	2.20	0.42
1:A:47:GLY:HA2	1:A:149:PRO:HD2	2.01	0.42
1:B:38:ALA:HB1	1:B:132:ILE:HG23	2.01	0.42
1:C:269:TYR:CE2	1:C:292:GLN:HG3	2.54	0.42
1:B:256:LEU:N	1:B:257:PRO:HD2	2.34	0.42
1:C:343:VAL:CG1	1:C:405:TYR:OH	2.68	0.42
1:A:223:PHE:CD1	1:A:228:VAL:HG21	2.54	0.42
1:C:223:PHE:CD1	1:C:228:VAL:HG21	2.55	0.42
1:D:399:VAL:O	1:D:399:VAL:CG2	2.68	0.42
1:A:325:HIS:CE1	1:B:384:ASP:OD1	2.73	0.42
1:A:100:PHE:CZ	1:A:126:THR:HG21	2.55	0.42
1:E:38:ALA:CB	1:E:132:ILE:HG23	2.49	0.42
4:B:612:HOH:O	1:D:312:ARG:HD3	2.19	0.42
1:D:59:ARG:HB3	1:D:123:LEU:HD23	2.01	0.42
1:A:253:HIS:HD2	1:A:255:ALA:HB3	1.86	0.41
1:C:121:LEU:HB3	1:C:132:ILE:CG1	2.50	0.41
1:C:278:ARG:NH2	1:C:420[A]:ARG:CD	2.83	0.41
1:D:100:PHE:CZ	1:D:126:THR:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HB3	1:A:357:TYR:CD1	2.56	0.41
1:D:155:VAL:HA	1:D:168:VAL:O	2.20	0.41
1:A:53:LEU:O	1:A:100:PHE:HA	2.21	0.41
1:A:304:ALA:O	1:A:320:GLY:HA3	2.21	0.41
1:A:390:THR:O	1:A:407:ARG:HB2	2.21	0.41
1:E:155:VAL:HA	1:E:168:VAL:O	2.21	0.41
1:E:230:GLU:CB	1:E:234:ARG:HH11	2.33	0.41
1:E:414:THR:HA	1:E:419:VAL:HG22	2.03	0.41
1:A:38:ALA:HB1	1:A:132:ILE:HG23	2.02	0.41
1:B:253:HIS:CD2	1:B:255:ALA:H	2.38	0.41
1:B:133:LEU:N	1:B:133:LEU:CD1	2.84	0.41
1:E:228:VAL:O	1:E:232:ILE:HG13	2.20	0.41
1:A:155:VAL:HA	1:A:168:VAL:O	2.21	0.41
1:A:256:LEU:N	1:A:257:PRO:HD2	2.35	0.41
1:B:59:ARG:HB3	1:B:123:LEU:HD23	2.02	0.41
1:C:150:GLU:H	1:C:150:GLU:HG2	1.81	0.41
1:C:44:ILE:HG23	1:C:96:ALA:HB3	2.03	0.41
1:C:390:THR:O	1:C:407:ARG:HB2	2.21	0.41
1:B:70:ILE:O	1:B:70:ILE:HG23	2.20	0.41
1:B:143:LEU:HD23	1:B:145:TYR:CZ	2.56	0.41
1:C:399:VAL:O	1:C:399:VAL:CG2	2.68	0.41
1:D:304:ALA:O	1:D:320:GLY:HA3	2.20	0.41
1:E:47:GLY:HA2	1:E:149:PRO:HD2	2.03	0.41
1:E:304:ALA:O	1:E:320:GLY:HA3	2.20	0.41
1:B:269:TYR:CE2	1:B:292:GLN:HG3	2.56	0.41
1:A:490:ARG:HG2	4:A:631:HOH:O	2.21	0.40
1:D:38:ALA:HB1	1:D:132:ILE:HG23	2.02	0.40
1:B:164:THR:HG21	1:B:363:ARG:HH12	1.86	0.40
1:A:269:TYR:CE2	1:A:292:GLN:HG3	2.57	0.40
1:B:155:VAL:HA	1:B:168:VAL:O	2.21	0.40
1:C:47:GLY:HA2	1:C:149:PRO:HD2	2.04	0.40
1:C:158:THR:HB	1:C:165:PRO:HA	2.02	0.40
1:D:47:GLY:HA2	1:D:149:PRO:HD2	2.04	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	A	481/499 (96%)	462 (96%)	18 (4%)	1 (0%)	43	72
1	B	477/499 (96%)	457 (96%)	15 (3%)	5 (1%)	12	38
1	C	484/499 (97%)	462 (96%)	20 (4%)	2 (0%)	30	60
1	D	481/499 (96%)	461 (96%)	16 (3%)	4 (1%)	16	44
1	E	479/499 (96%)	464 (97%)	13 (3%)	2 (0%)	30	60
All	All	2402/2495 (96%)	2306 (96%)	82 (3%)	14 (1%)	21	51

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	444	ASP
1	C	444	ASP
1	D	444	ASP
1	A	444	ASP
1	B	44	ILE
1	D	44	ILE
1	E	165	PRO
1	D	165	PRO
1	B	166	LYS
1	D	166	LYS
1	B	165	PRO
1	C	324	PRO
1	E	342	ALA
1	B	11	ILE

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	A	347/384 (90%)	320 (92%)	27 (8%)	11	35
1	B	263/384 (68%)	233 (89%)	30 (11%)	5	19
1	E	157/384 (41%)	139 (88%)	18 (12%)	5	18
All	All	767/1152 (67%)	692 (90%)	75 (10%)	7	25

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	40	THR
1	A	126	THR
1	A	150	GLU
1	A	192	ARG
1	A	194	LEU
1	A	195	ILE
1	A	226	ASP
1	A	236	ARG
1	A	245	ASN
1	A	266	ARG
1	A	278	ARG
1	A	286	MET
1	A	290	LEU
1	A	296	THR
1	A	314	GLU
1	A	350	SER
1	A	366	GLN
1	A	367	VAL
1	A	391	ASP
1	A	399	VAL
1	A	414	THR
1	A	420	ARG
1	A	442	VAL
1	A	468	ARG
1	A	480	PRO
1	A	487	VAL
1	B	9	ASP
1	B	40	THR
1	B	70	ILE
1	B	84	THR

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Mol	Chain	Res	Type
1	B	85	GLU
1	B	126	THR
1	B	128	ARG
1	B	133	LEU
1	B	147	GLU
1	B	150	GLU
1	B	158	THR
1	B	164	THR
1	B	184	SER
1	B	188	ARG
1	B	194	LEU
1	B	196	PRO
1	B	197	ILE
1	B	226	ASP
1	B	229	LEU
1	B	236	ARG
1	B	245	ASN
1	B	266	ARG
1	B	278	ARG
1	B	286	MET
1	B	290	LEU
1	B	313	ARG
1	B	314	GLU
1	B	350	SER
1	B	360	ASP
1	B	367	VAL
1	E	286	MET
1	E	290	LEU
1	E	314	GLU
1	E	350	SER
1	E	367	VAL
1	E	391	ASP
1	E	393	LEU
1	E	400	GLU
1	E	413	LEU
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	480	PRO

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Mol	Chain	Res	Type
1	E	487	VAL
1	E	490	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	54	HIS
1	A	170	HIS
1	A	208	GLN
1	A	253	HIS
1	A	293	ASN
1	A	366	GLN
1	A	386	HIS
1	A	388	HIS
1	A	452	HIS
1	A	465	HIS
1	B	54	HIS
1	B	170	HIS
1	B	208	GLN
1	B	253	HIS
1	B	293	ASN
1	B	386	HIS
1	E	293	ASN
1	E	297	GLN
1	E	386	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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
2	AMP	D	501	-	25,25,25	1.41	3 (12%)	37,38,38	2.06	12 (32%)
3	EQ2	E	502	-	20,21,21	0.69	0	29,31,31	0.87	1 (3%)
2	AMP	A	501	-	25,25,25	1.82	6 (24%)	37,38,38	1.72	10 (27%)
3	EQ2	C	502	-	20,21,21	0.81	1 (5%)	29,31,31	0.91	1 (3%)
2	AMP	E	501	-	21,21,25	2.10	5 (23%)	31,31,38	1.97	9 (29%)
3	EQ2	B	502	-	20,21,21	0.70	0	29,31,31	0.86	0
2	AMP	C	501	-	25,25,25	1.70	4 (16%)	37,38,38	2.20	13 (35%)
2	AMP	B	501	-	25,25,25	1.58	7 (28%)	37,38,38	2.37	14 (37%)
3	EQ2	A	502	-	20,21,21	0.67	0	29,31,31	1.12	2 (6%)
3	EQ2	D	502	-	20,21,21	0.68	1 (5%)	29,31,31	1.02	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AMP	D	501	-	-	3/10/26/26	0/3/3/3
3	EQ2	E	502	-	-	4/8/8/8	0/3/3/3
2	AMP	A	501	-	-	2/10/26/26	0/3/3/3
3	EQ2	C	502	-	-	4/8/8/8	0/3/3/3
2	AMP	E	501	-	-	1/6/22/26	0/3/3/3
3	EQ2	B	502	-	-	5/8/8/8	0/3/3/3
2	AMP	C	501	-	-	5/10/26/26	0/3/3/3
2	AMP	B	501	-	-	5/10/26/26	0/3/3/3
3	EQ2	A	502	-	-	4/8/8/8	0/3/3/3
3	EQ2	D	502	-	-	4/8/8/8	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	501	AMP	C5-C4	6.62	1.50	1.39
2	A	501	AMP	C5-C4	6.19	1.50	1.39
2	C	501	AMP	C5-C4	5.49	1.48	1.39
2	D	501	AMP	C5-C4	4.04	1.46	1.39
2	B	501	AMP	C5-C4	3.33	1.45	1.39
2	C	501	AMP	C8-N7	3.23	1.37	1.31
2	D	501	AMP	C4-N9	-3.17	1.31	1.37
2	B	501	AMP	C8-N9	-3.13	1.32	1.37
2	B	501	AMP	C5-N7	-3.06	1.33	1.39
2	C	501	AMP	C5-C6	3.02	1.49	1.41
2	E	501	AMP	O4'-C1'	2.97	1.48	1.42
2	E	501	AMP	C8-N7	2.93	1.37	1.31
2	A	501	AMP	C4-N9	-2.88	1.31	1.37
2	A	501	AMP	C2-N1	2.85	1.39	1.33
2	B	501	AMP	C5-C6	2.63	1.48	1.41
2	A	501	AMP	C8-N7	2.54	1.36	1.31
3	C	502	EQ2	O2-C5	-2.47	1.23	1.30
2	D	501	AMP	C8-N7	2.46	1.36	1.31
2	E	501	AMP	C4-N3	2.34	1.38	1.34
2	A	501	AMP	C5-C6	2.29	1.47	1.41
3	D	502	EQ2	O2-C5	-2.23	1.23	1.30
2	B	501	AMP	C8-N7	2.23	1.36	1.31
2	B	501	AMP	C4-N9	-2.22	1.33	1.37
2	A	501	AMP	C5-N7	-2.21	1.35	1.39
2	E	501	AMP	C5-C6	2.17	1.47	1.41
2	C	501	AMP	C4-N9	-2.16	1.33	1.37
2	B	501	AMP	P-O5'	2.08	1.66	1.60

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	C5-C4-N3	-5.63	118.96	126.72
2	D	501	AMP	C4-N9-C8	5.42	111.43	105.74
2	C	501	AMP	C5-C4-N3	-5.35	119.35	126.72
2	B	501	AMP	C4-C5-N7	-5.10	104.75	110.58
2	C	501	AMP	N3-C2-N1	-4.85	121.23	128.58
2	E	501	AMP	N3-C2-N1	-4.64	121.56	128.58
2	E	501	AMP	C2-N1-C6	4.41	125.98	118.73
2	D	501	AMP	N3-C4-N9	4.33	134.52	127.17
2	C	501	AMP	C2-N3-C4	4.30	122.34	111.83
2	C	501	AMP	N3-C4-N9	4.25	134.39	127.17
2	B	501	AMP	C5-N7-C8	4.02	109.77	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	AMP	N3-C4-N9	4.00	133.97	127.17
2	B	501	AMP	C2-N3-C4	3.98	121.55	111.83
2	A	501	AMP	C4-N9-C8	3.89	109.83	105.74
2	B	501	AMP	N3-C2-N1	-3.89	122.69	128.58
2	E	501	AMP	N3-C4-N9	3.74	133.53	127.17
2	D	501	AMP	C5-C4-N3	-3.71	121.60	126.72
2	B	501	AMP	C4-N9-C8	3.68	109.61	105.74
2	B	501	AMP	N9-C8-N7	-3.61	108.81	113.94
2	C	501	AMP	C2'-C1'-N9	-3.49	104.64	113.30
2	B	501	AMP	C2'-C1'-N9	-3.40	104.86	113.30
2	A	501	AMP	N3-C4-N9	3.32	132.81	127.17
2	B	501	AMP	C6-C5-N7	3.29	138.44	132.09
2	C	501	AMP	C4-N9-C8	3.26	109.16	105.74
3	A	502	EQ2	O3-C5-C4	-3.25	114.75	121.30
2	A	501	AMP	C4'-O4'-C1'	-3.25	102.29	109.47
2	E	501	AMP	C5-C4-N3	-3.23	122.27	126.72
2	D	501	AMP	O3P-P-O2P	3.23	119.92	107.80
2	D	501	AMP	N3-C2-N1	-3.11	123.88	128.58
2	C	501	AMP	C4-C5-N7	-2.97	107.19	110.58
2	D	501	AMP	O3P-P-O5'	-2.95	98.97	106.67
2	A	501	AMP	N6-C6-N1	2.86	124.75	118.38
2	E	501	AMP	C2-N3-C4	2.85	118.79	111.83
2	C	501	AMP	C6-C5-N7	2.83	137.54	132.09
2	D	501	AMP	C2-N3-C4	2.76	118.56	111.83
2	D	501	AMP	N9-C8-N7	-2.75	110.04	113.94
2	A	501	AMP	C4-N9-C1'	-2.72	120.27	126.63
2	E	501	AMP	C4-N9-C8	2.68	108.55	105.74
2	C	501	AMP	C2-N1-C6	2.62	123.04	118.73
2	D	501	AMP	C5-C6-N6	-2.55	116.96	123.29
2	E	501	AMP	N6-C6-N1	2.55	124.05	118.38
2	A	501	AMP	O4'-C1'-N9	2.54	112.96	108.09
2	D	501	AMP	O2P-P-O5'	-2.48	100.19	106.67
2	E	501	AMP	O2'-C2'-C1'	-2.46	101.62	110.10
2	E	501	AMP	O2'-C2'-C3'	2.46	119.71	111.82
2	A	501	AMP	C2-N1-C6	2.46	122.77	118.73
2	B	501	AMP	C4-N9-C1'	-2.43	120.94	126.63
2	B	501	AMP	O2P-P-O5'	-2.40	100.41	106.67
2	D	501	AMP	N6-C6-N1	2.37	123.66	118.38
3	D	502	EQ2	O3-C5-C4	-2.35	116.57	121.30
2	A	501	AMP	C5-C4-N3	-2.32	123.52	126.72
2	B	501	AMP	O3P-P-O2P	2.30	116.44	107.80
2	A	501	AMP	C2'-C1'-N9	-2.29	107.61	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	AMP	C2'-C3'-C4'	2.26	106.97	102.61
2	C	501	AMP	O4'-C1'-N9	2.20	112.31	108.09
3	A	502	EQ2	O2-C5-C4	2.19	119.91	114.71
2	B	501	AMP	O4'-C1'-N9	2.18	112.28	108.09
3	E	502	EQ2	O3-C5-C4	-2.09	117.09	121.30
3	C	502	EQ2	C7-C14-C3	-2.06	118.59	120.10
2	C	501	AMP	O3P-P-O5'	-2.06	101.29	106.67
2	D	501	AMP	O4'-C1'-C2'	2.05	111.00	106.62
2	C	501	AMP	N9-C8-N7	-2.02	111.07	113.94
2	A	501	AMP	N3-C2-N1	-2.00	125.55	128.58

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	AMP	C5'-O5'-P-O1P
2	C	501	AMP	C5'-O5'-P-O2P
2	C	501	AMP	C5'-O5'-P-O3P
2	D	501	AMP	C5'-O5'-P-O2P
2	D	501	AMP	C5'-O5'-P-O3P
3	A	502	EQ2	C1-C2-C3-N1
3	A	502	EQ2	O1-C2-C3-N1
3	B	502	EQ2	C1-C2-C3-N1
3	B	502	EQ2	C1-C2-C3-C14
3	B	502	EQ2	O1-C2-C3-N1
3	B	502	EQ2	O1-C2-C3-C14
3	C	502	EQ2	C1-C2-C3-C14
3	C	502	EQ2	O1-C2-C3-C14
3	E	502	EQ2	C1-C2-C3-N1
3	E	502	EQ2	O1-C2-C3-N1
2	A	501	AMP	O4'-C4'-C5'-O5'
2	A	501	AMP	C3'-C4'-C5'-O5'
2	C	501	AMP	O4'-C4'-C5'-O5'
2	C	501	AMP	C3'-C4'-C5'-O5'
3	A	502	EQ2	C1-C2-C3-C14
3	E	502	EQ2	C1-C2-C3-C14
3	E	502	EQ2	O1-C2-C3-C14
3	C	502	EQ2	O1-C2-C3-N1
2	B	501	AMP	C5'-O5'-P-O3P
2	C	501	AMP	C4'-C5'-O5'-P
3	D	502	EQ2	C1-C2-C3-C14
3	D	502	EQ2	O1-C2-C3-C14

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Mol	Chain	Res	Type	Atoms
2	B	501	AMP	C3'-C4'-C5'-O5'
3	C	502	EQ2	C1-C2-C3-N1
3	D	502	EQ2	C1-C2-C3-N1
3	D	502	EQ2	O1-C2-C3-N1
2	B	501	AMP	O4'-C4'-C5'-O5'
2	E	501	AMP	O4'-C4'-C5'-O5'
3	B	502	EQ2	N1-C4-C5-O2
2	B	501	AMP	C5'-O5'-P-O2P
2	D	501	AMP	C5'-O5'-P-O1P
3	A	502	EQ2	O1-C2-C3-C14

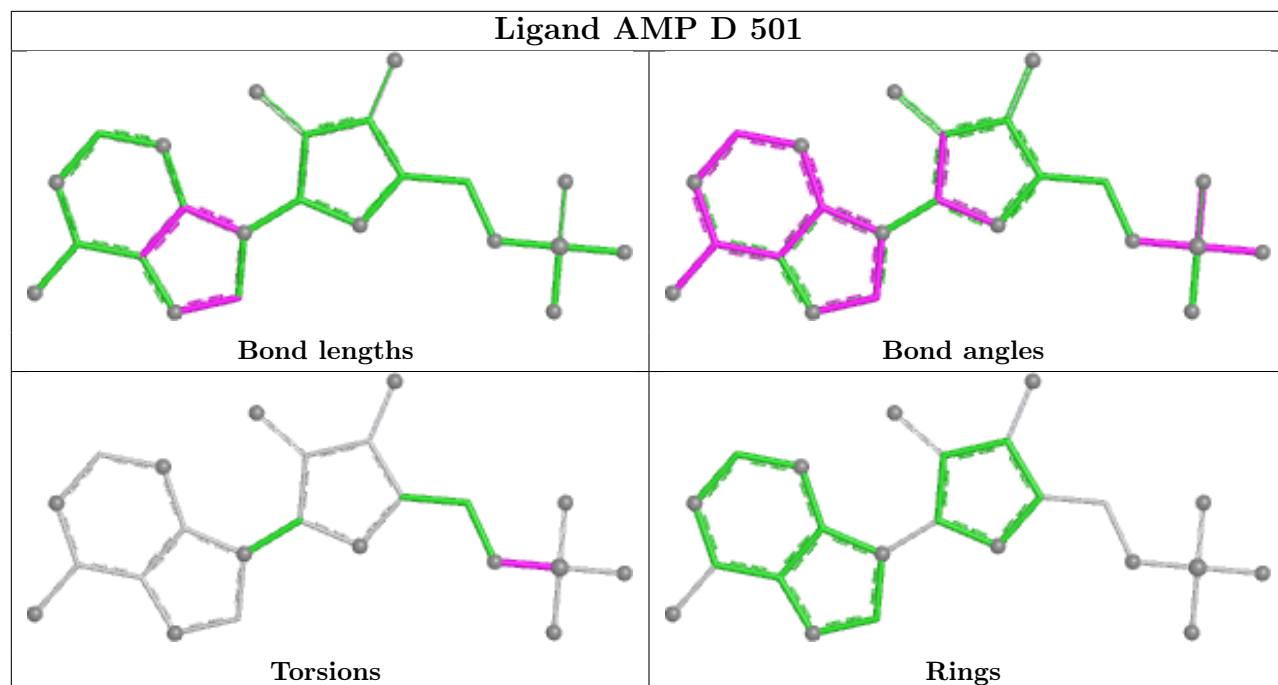
There are no ring outliers.

6 monomers are involved in 8 short contacts:

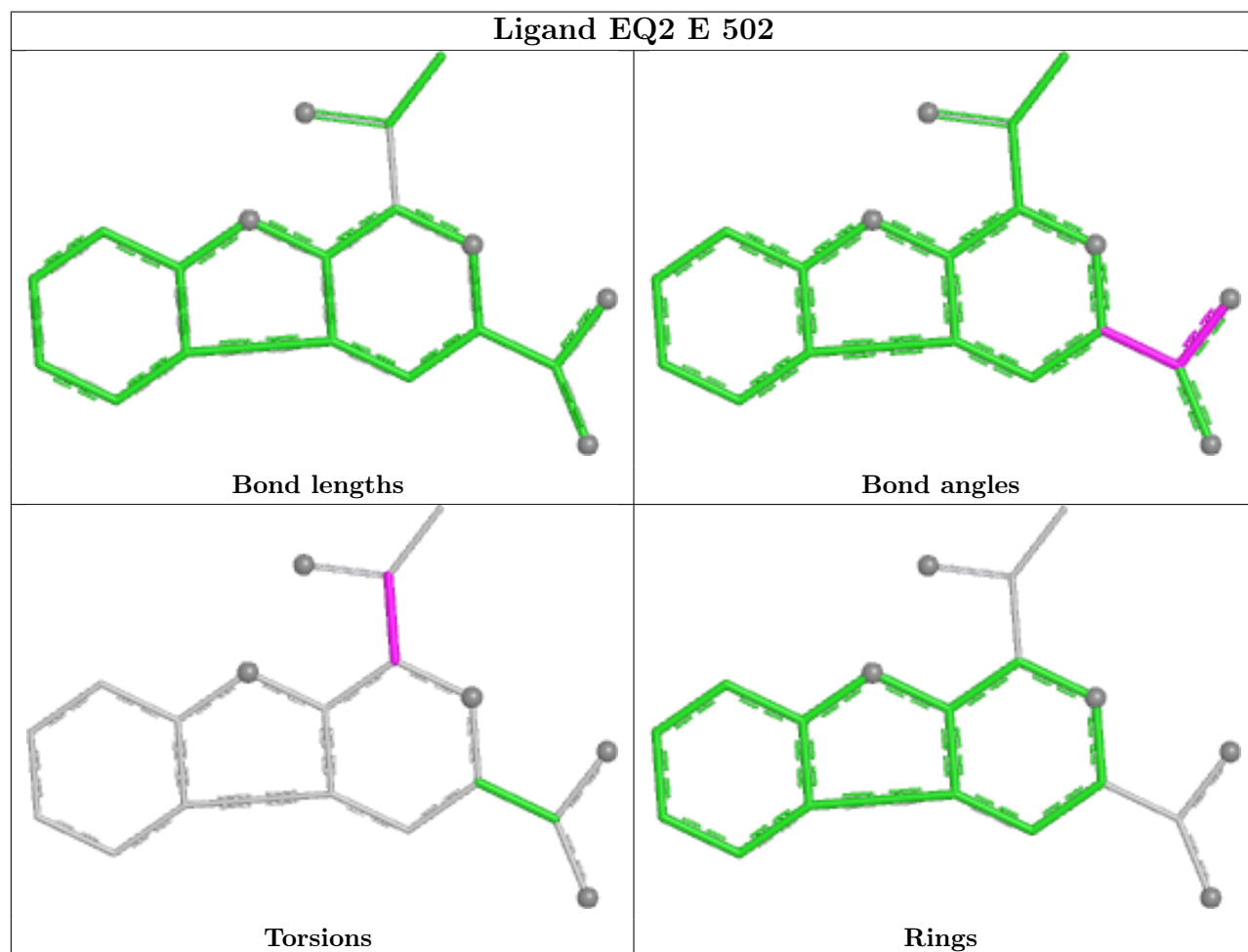
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	AMP	1	0
2	A	501	AMP	1	0
3	C	502	EQ2	1	0
2	E	501	AMP	1	0
2	C	501	AMP	2	0
2	B	501	AMP	2	0

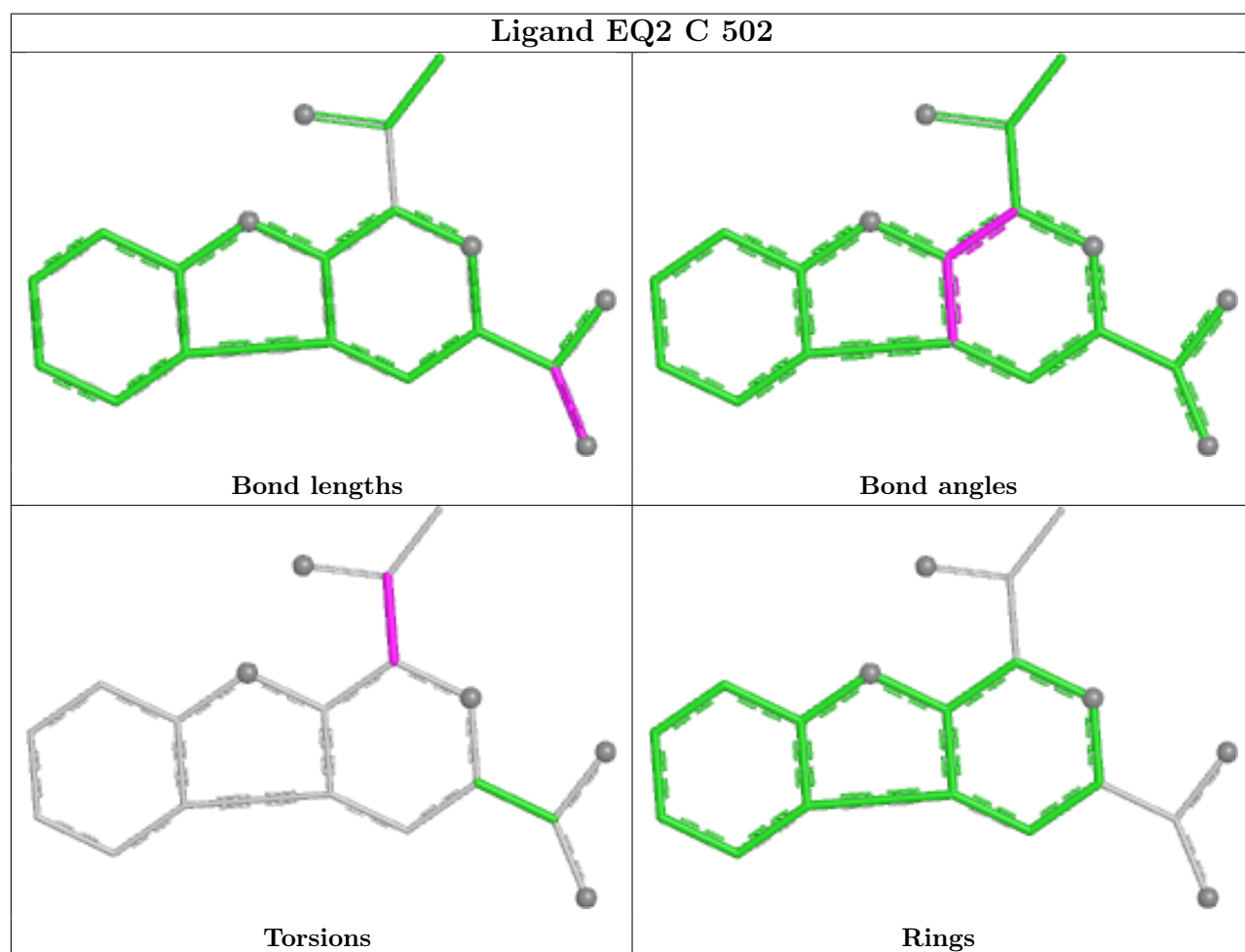
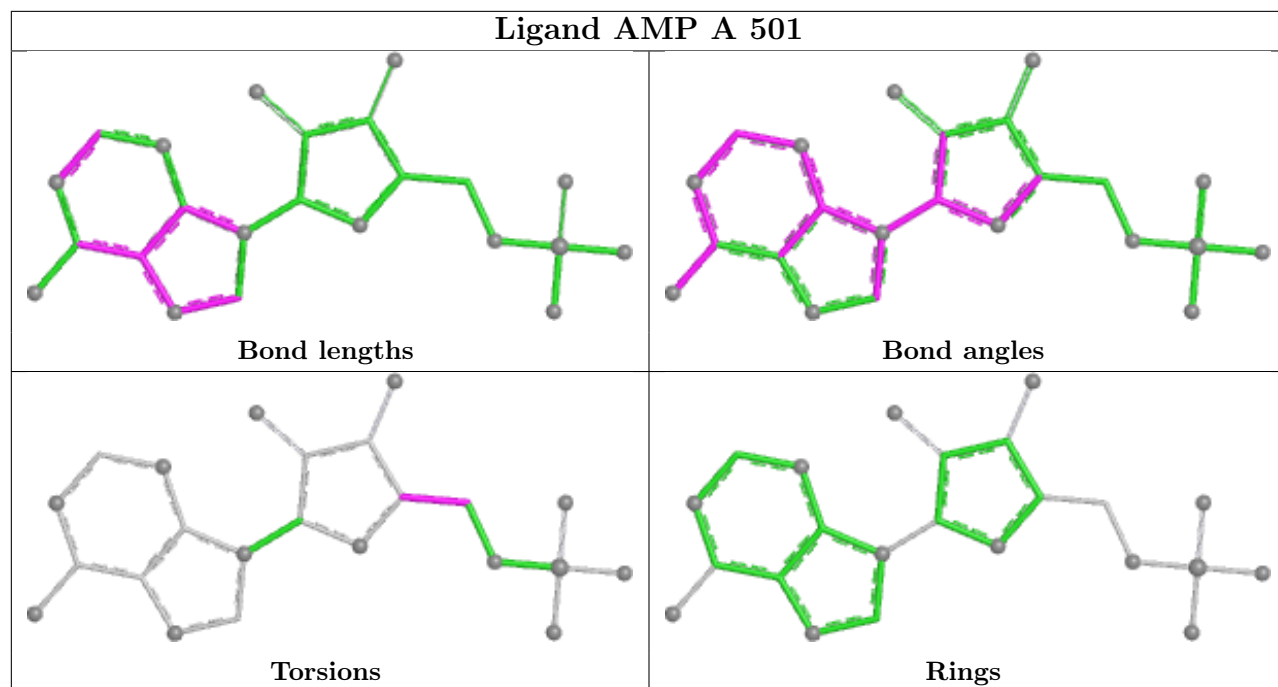
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

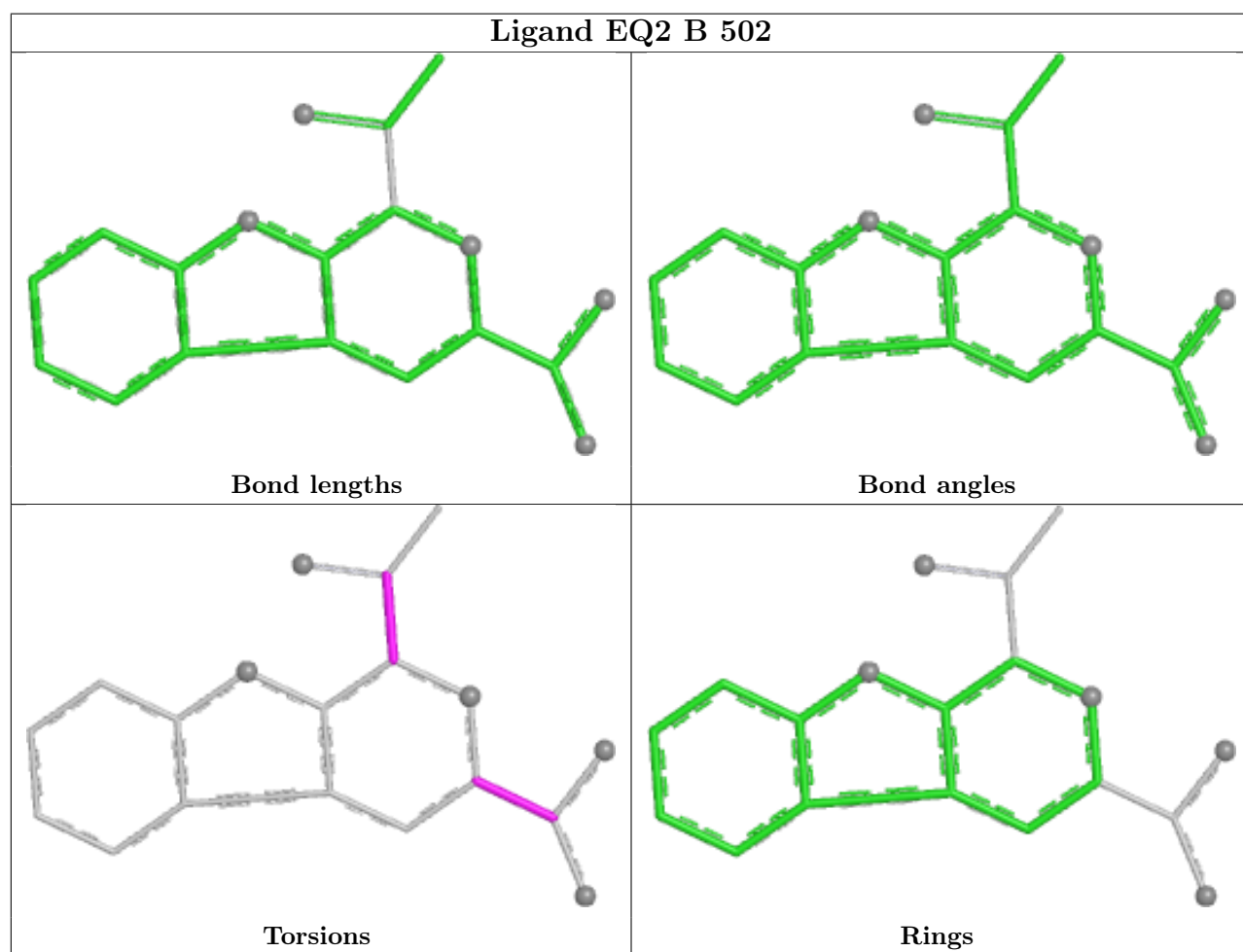
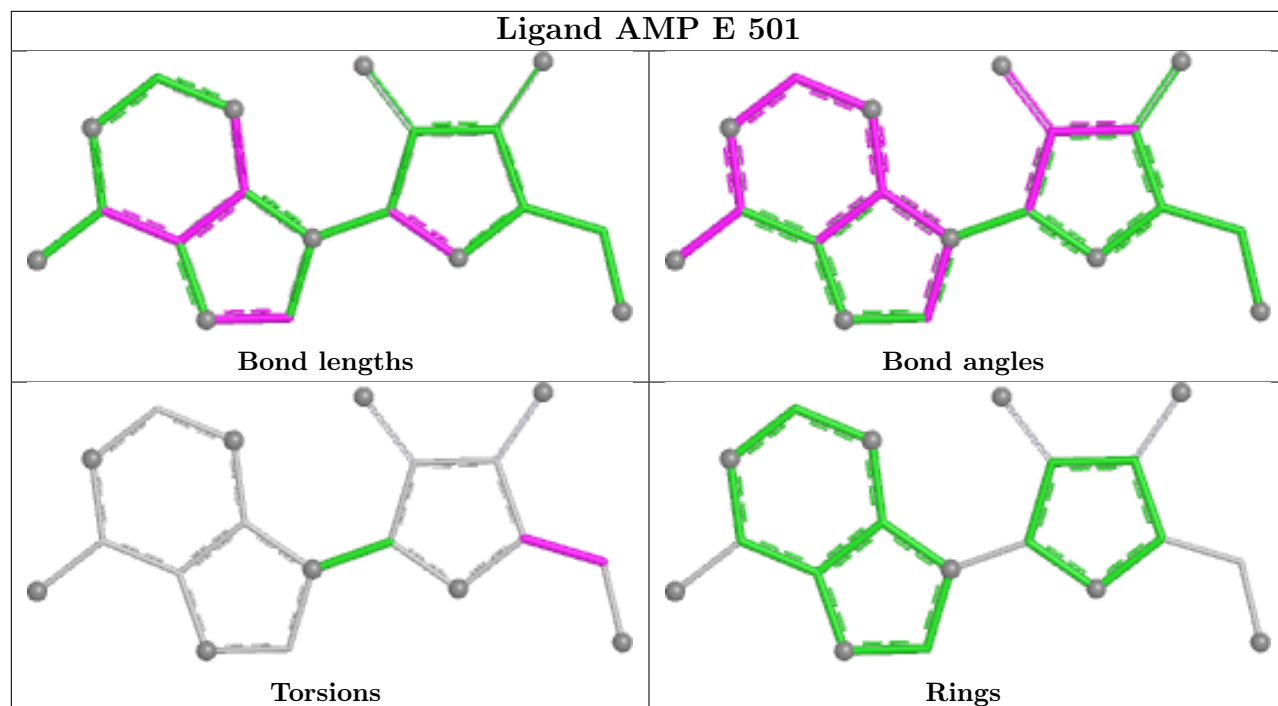
Ligand AMP D 501

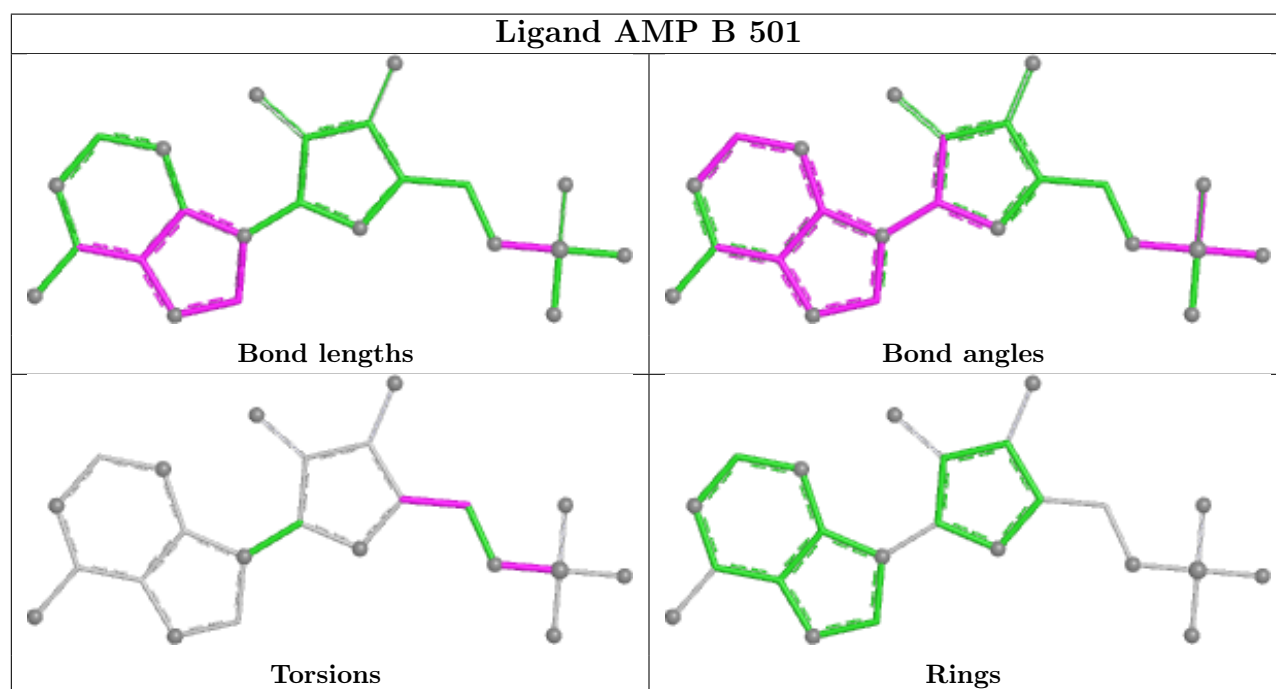
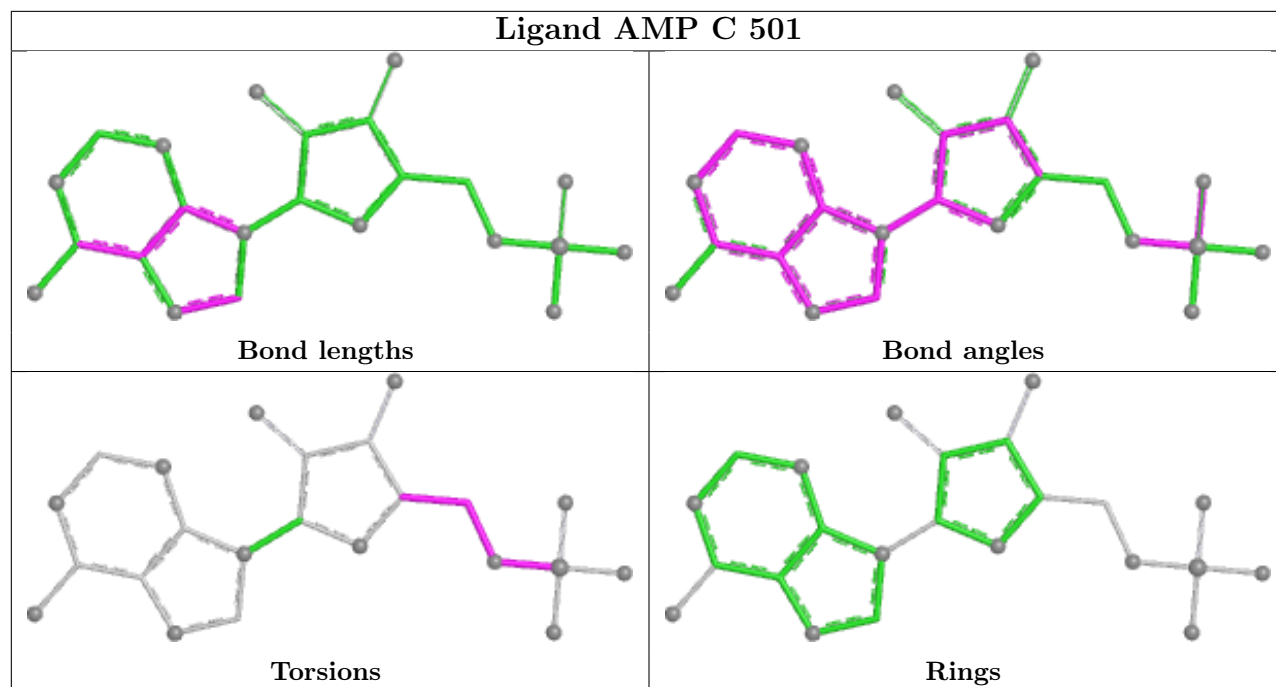


Ligand EQ2 E 502

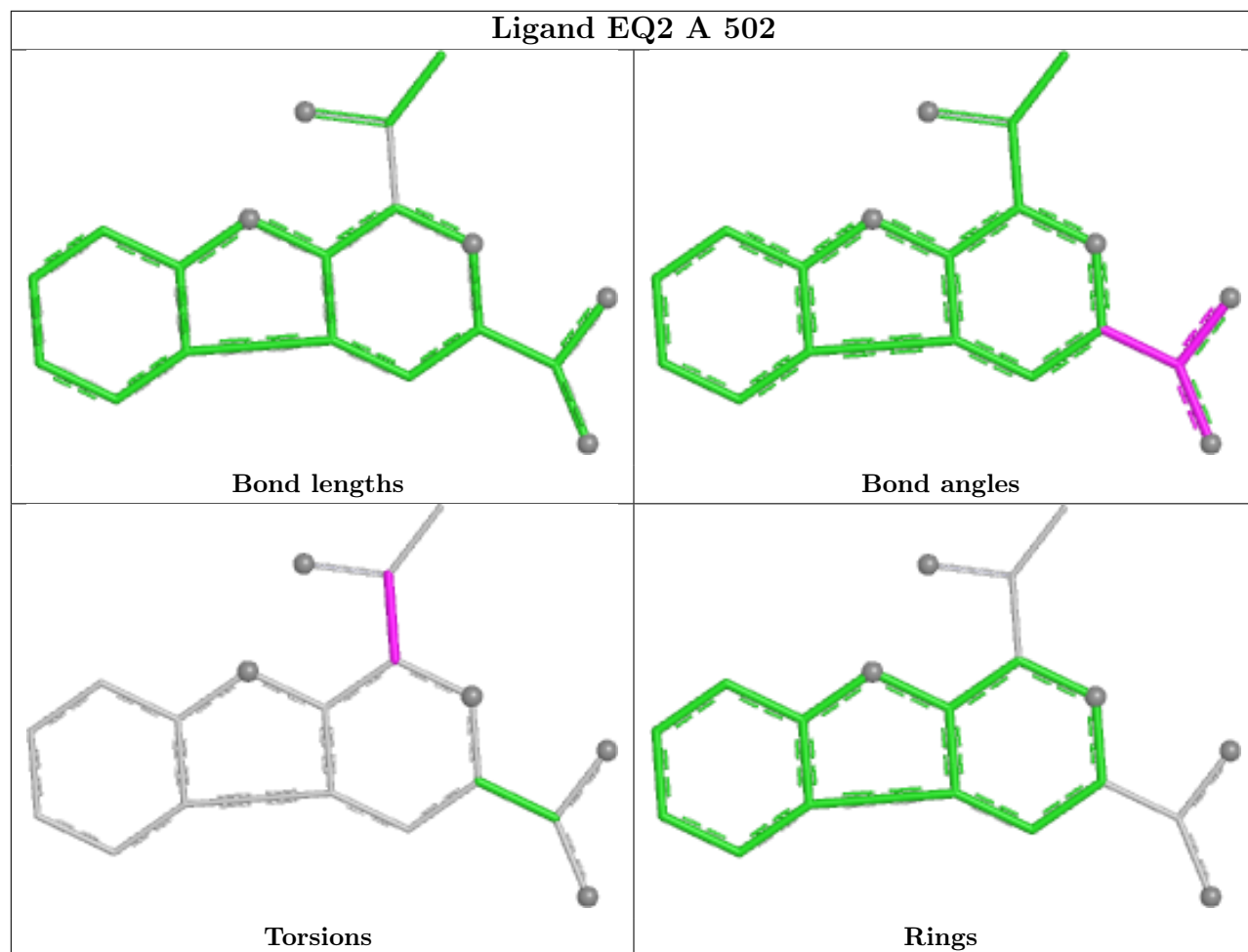


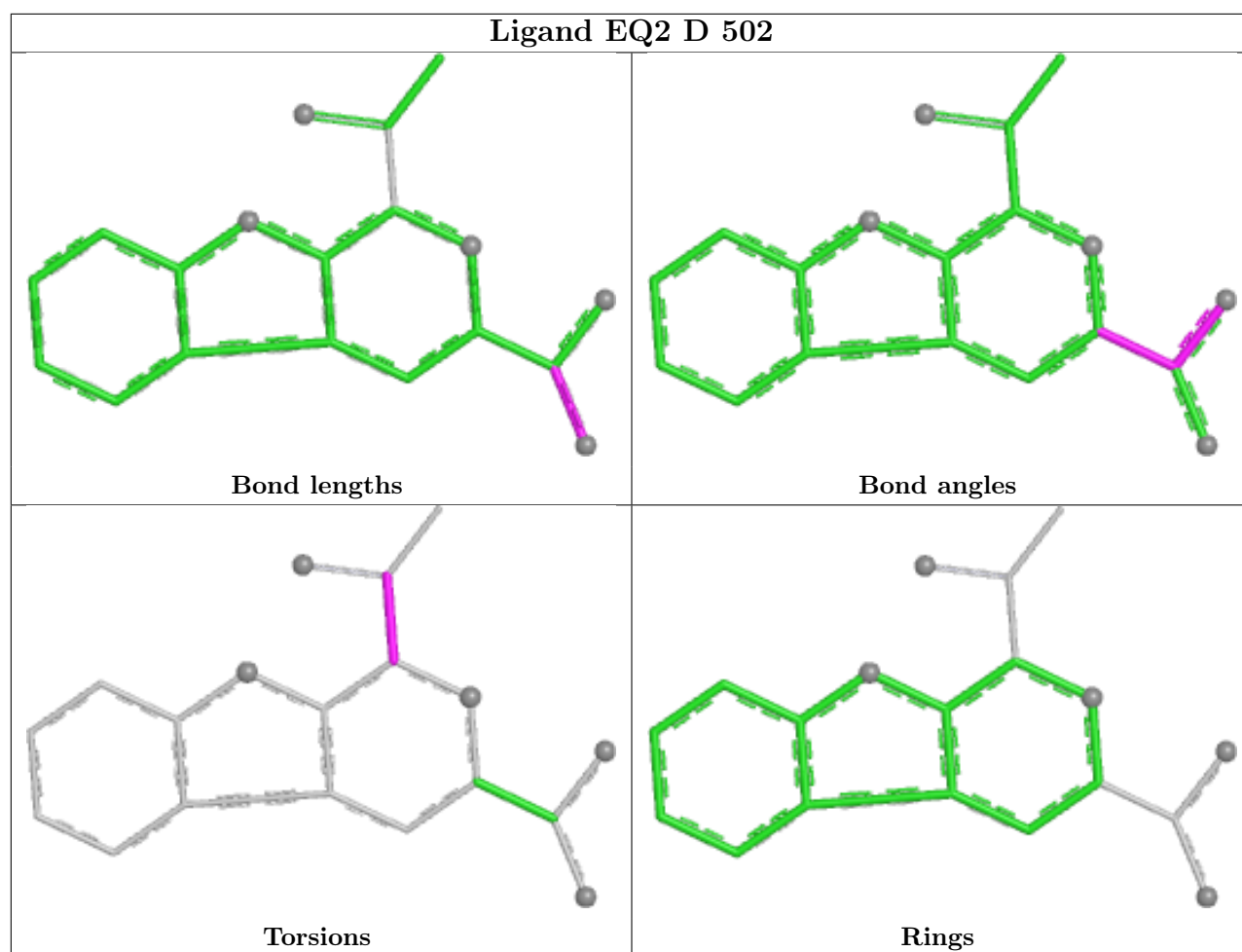






Ligand EQ2 A 502





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	487/499 (97%)	-0.05	8 (1%) 70 61	23, 46, 75, 100	0
1	B	485/499 (97%)	-0.02	9 (1%) 66 57	26, 47, 76, 121	0
1	C	490/499 (98%)	0.12	20 (4%) 41 33	15, 49, 89, 117	2 (0%)
1	D	487/499 (97%)	-0.02	2 (0%) 88 84	23, 47, 80, 115	0
1	E	487/499 (97%)	0.30	15 (3%) 51 41	39, 61, 96, 126	0
All	All	2436/2495 (97%)	0.06	54 (2%) 62 52	15, 51, 85, 126	2 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	119	VAL	3.8
1	C	134	ALA	3.8
1	A	165	PRO	3.7
1	E	418	ASP	3.5
1	B	163	GLY	3.3
1	E	42	ALA	3.2
1	C	160	GLY	3.2
1	C	127	SER	3.2
1	E	117	VAL	3.0
1	C	138	PRO	3.0
1	E	444	ASP	3.0
1	E	446	ALA	2.8
1	C	77	LEU	2.8
1	A	19	ALA	2.8
1	C	158	THR	2.8
1	C	128	ARG	2.7
1	E	443	ALA	2.6
1	B	165	PRO	2.5
1	B	432	SER	2.5
1	C	112	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	129	GLY	2.4
1	A	113	GLU	2.4
1	E	479	THR	2.4
1	A	138	PRO	2.4
1	A	116	SER	2.4
1	C	190	PRO	2.3
1	C	18	GLY	2.3
1	E	230	GLU	2.3
1	A	48	ARG	2.3
1	C	165	PRO	2.3
1	B	483	ALA	2.3
1	E	495	ASP	2.3
1	E	16	VAL	2.2
1	C	111	LEU	2.2
1	C	141	THR	2.2
1	C	494	THR	2.2
1	B	18	GLY	2.2
1	B	341	GLY	2.2
1	A	339	PRO	2.2
1	E	308	ASP	2.2
1	C	38	ALA	2.2
1	C	137	VAL	2.1
1	B	431	ASP	2.1
1	B	80	THR	2.1
1	C	-1	PRO	2.1
1	C	142	PRO	2.1
1	D	18	GLY	2.1
1	E	205	GLU	2.1
1	E	448	PRO	2.1
1	B	335	GLY	2.1
1	E	132	ILE	2.1
1	D	480	PRO	2.0
1	E	258	ARG	2.0
1	C	60	ALA	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

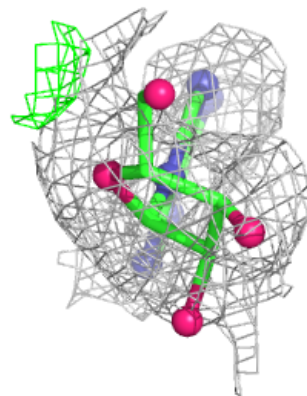
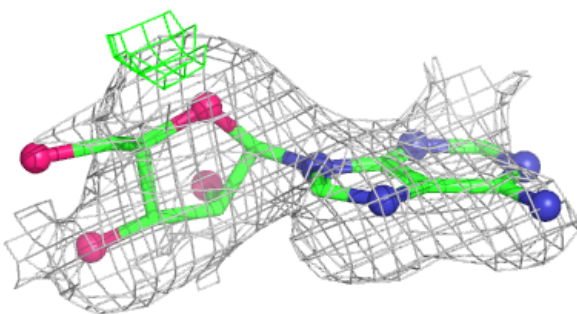
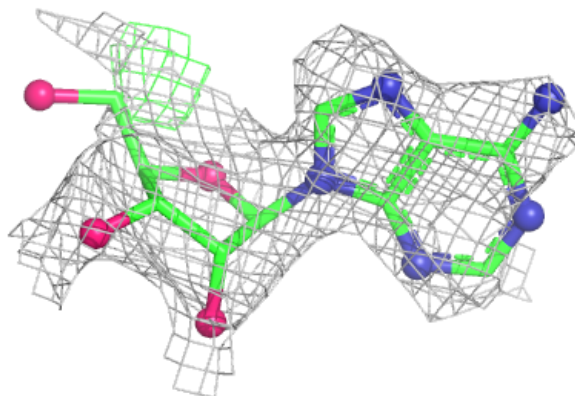
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	E	501	19/23	0.90	0.09	46,51,57,57	0
3	EQ2	E	502	19/19	0.93	0.11	53,55,80,86	0
2	AMP	C	501	23/23	0.94	0.09	37,41,56,58	0
2	AMP	B	501	23/23	0.96	0.06	36,40,55,61	0
2	AMP	D	501	23/23	0.96	0.07	36,41,53,60	0
3	EQ2	A	502	19/19	0.97	0.08	39,44,52,63	0
3	EQ2	B	502	19/19	0.97	0.07	37,41,50,55	0
3	EQ2	C	502	19/19	0.97	0.07	40,43,49,49	0
3	EQ2	D	502	19/19	0.97	0.08	37,40,45,50	0
2	AMP	A	501	23/23	0.97	0.06	36,42,52,58	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.

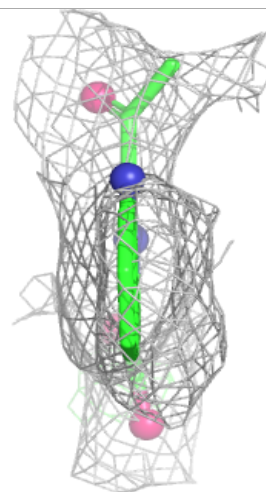
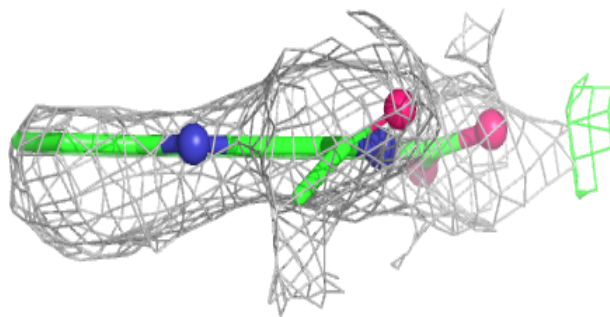
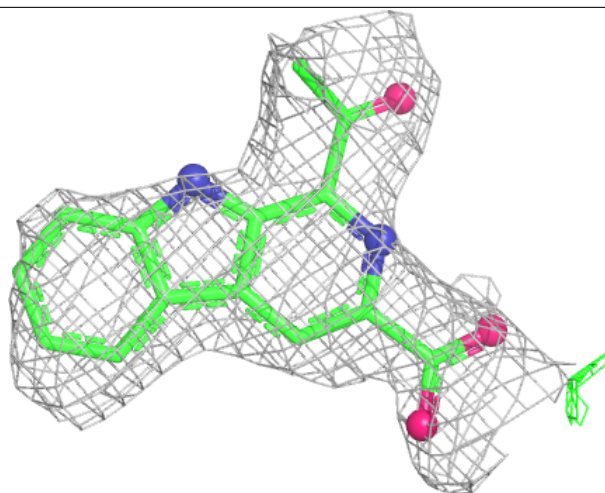
Electron density around AMP E 501:

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



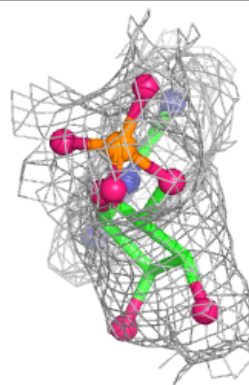
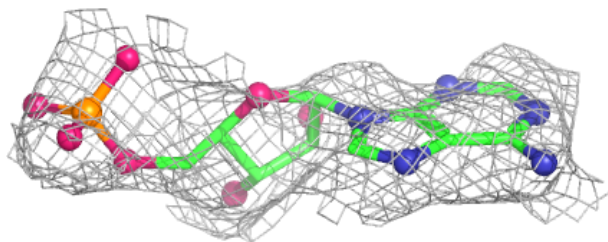
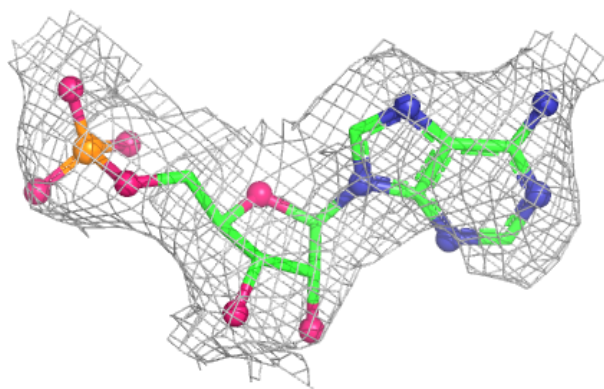
Electron density around EQ2 E 502:

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

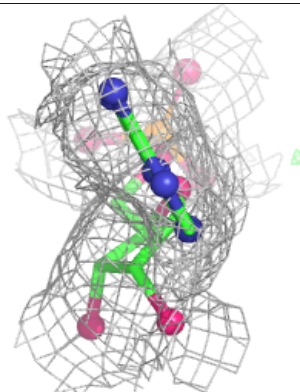
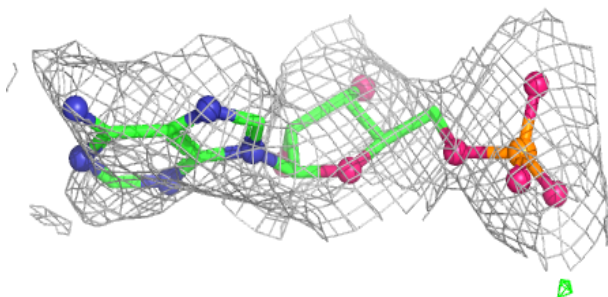
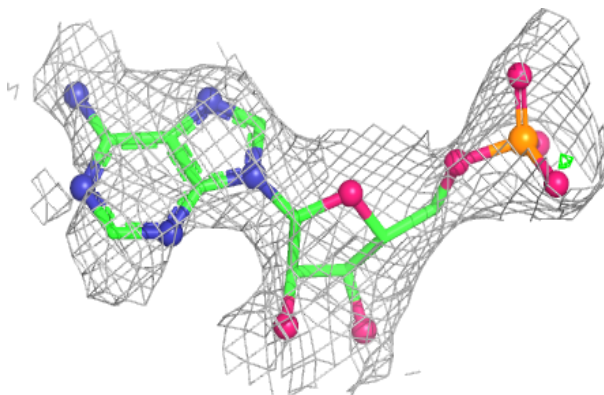


Electron density around AMP C 501:

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

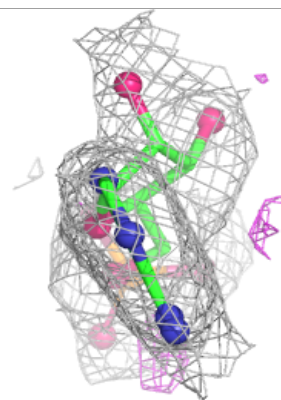
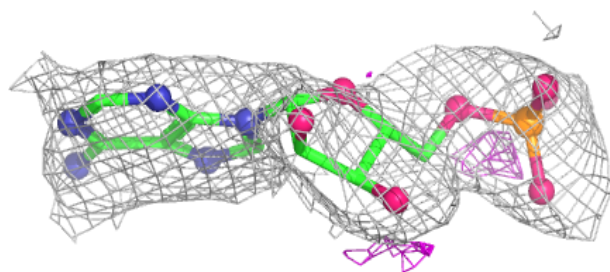
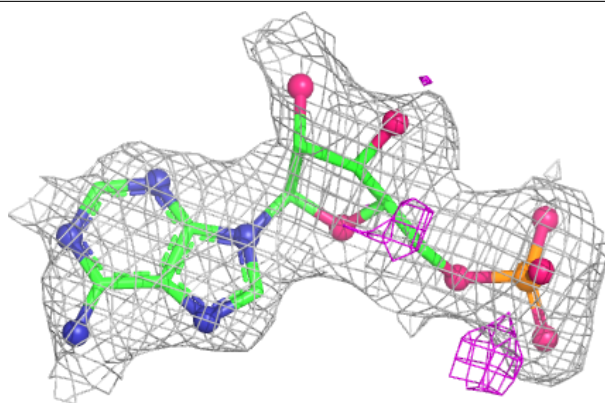
**Electron density around AMP B 501:**

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



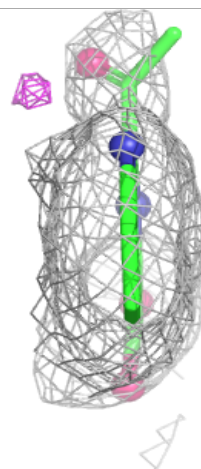
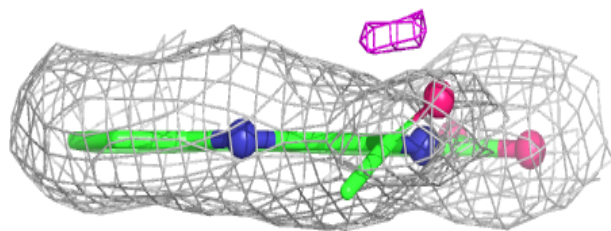
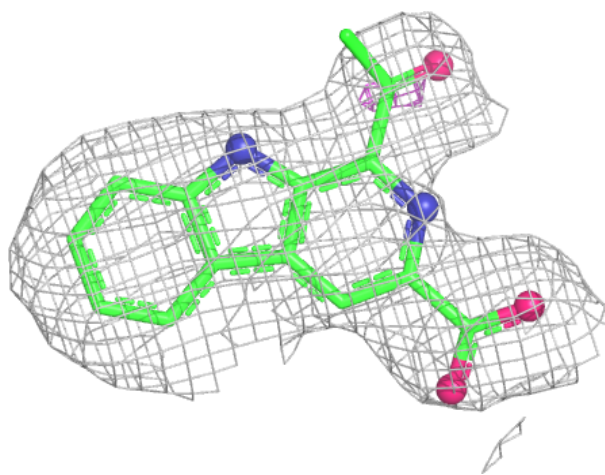
Electron density around AMP D 501:

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



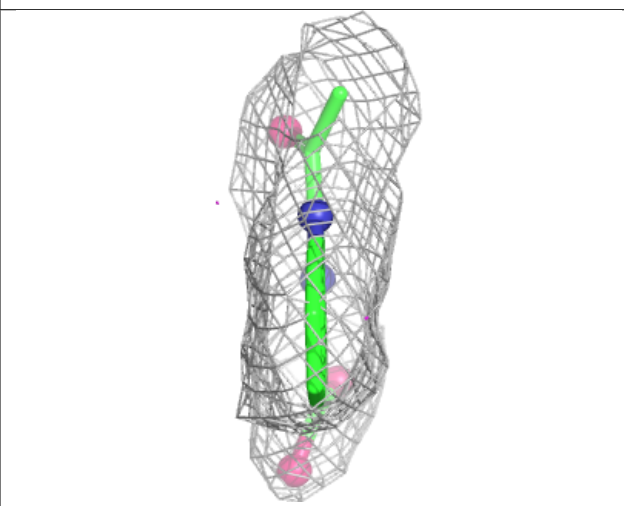
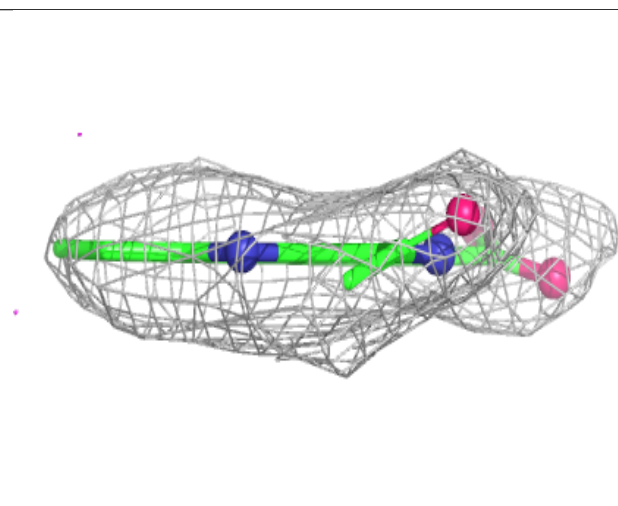
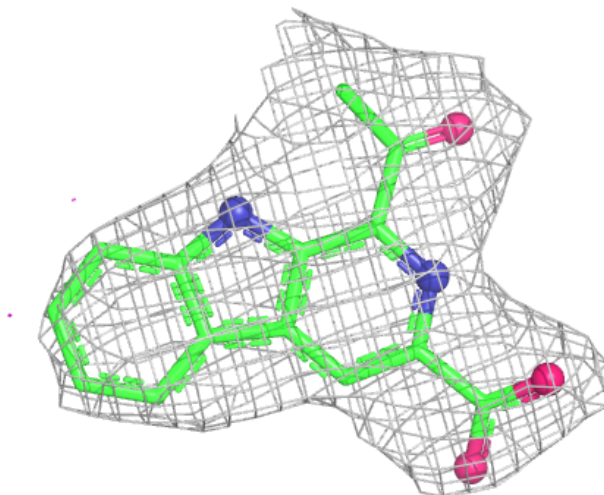
Electron density around EQ2 A 502:

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and green (positive)



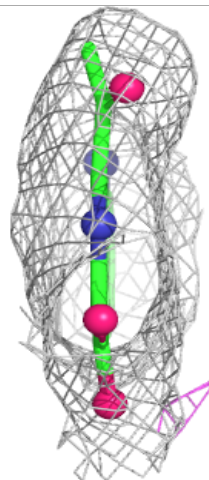
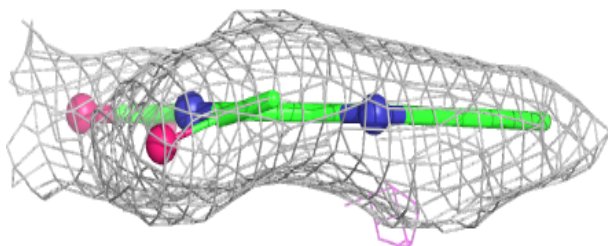
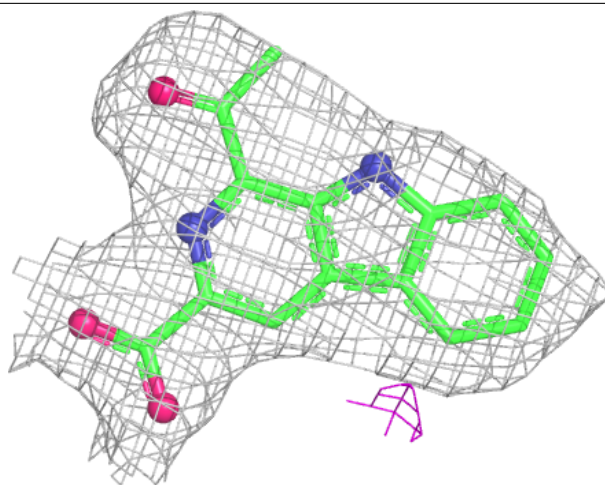
Electron density around EQ2 B 502:

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



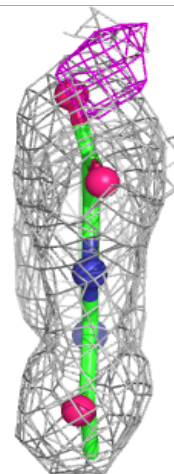
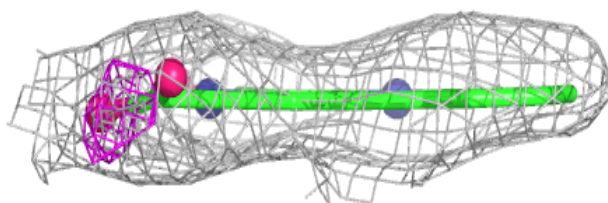
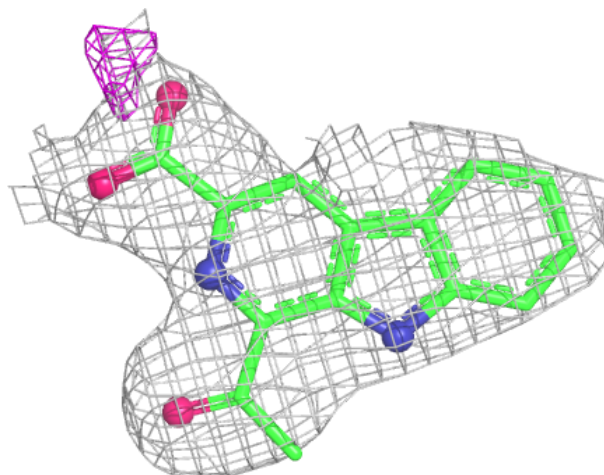
Electron density around EQ2 C 502:

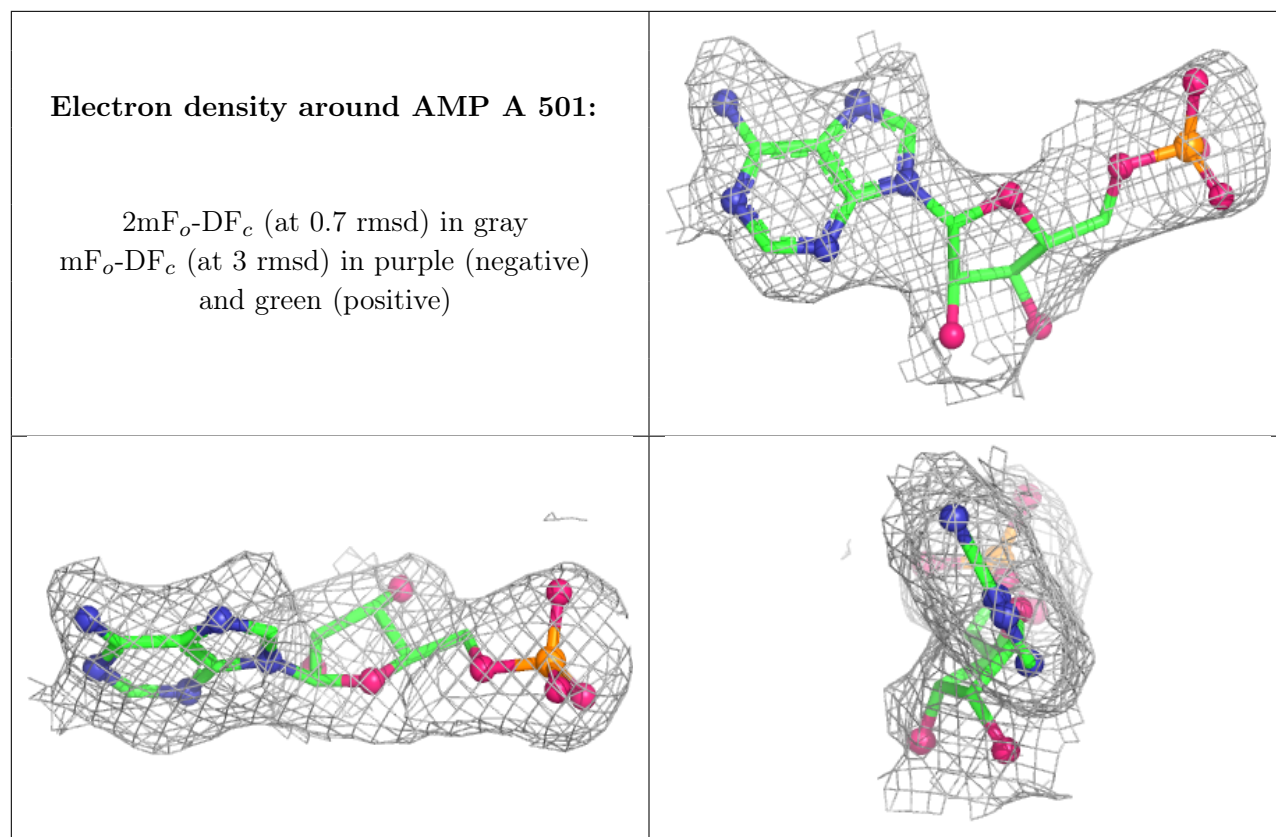
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around EQ2 D 502:

$2mF_o-DF_c$ (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.