



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 05:29 PM UTC

PDB ID : 6SQ8 / pdb_00006sq8
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	:	4-5-2 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

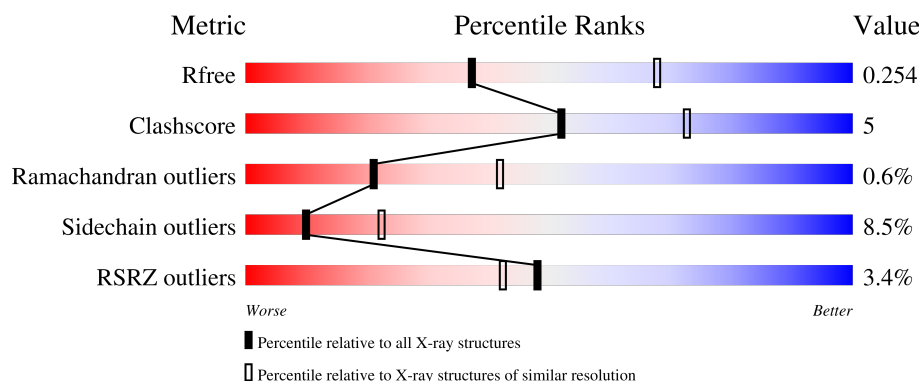
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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	3% 85% 10% ..
1	B	498	4% 84% 13% ...
1	C	498	3% 82% 12% ..
1	D	498	3% 82% 12% ..
1	E	498	5% 82% 15% ..

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.

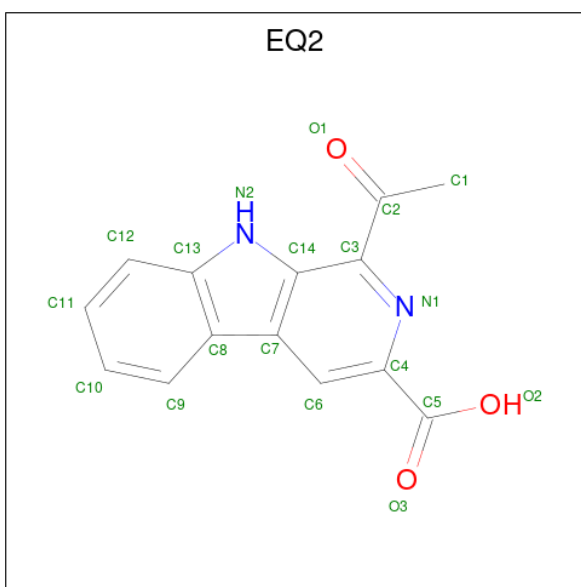
- Molecule 1 is a protein called Fatty acid CoA ligase.

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:

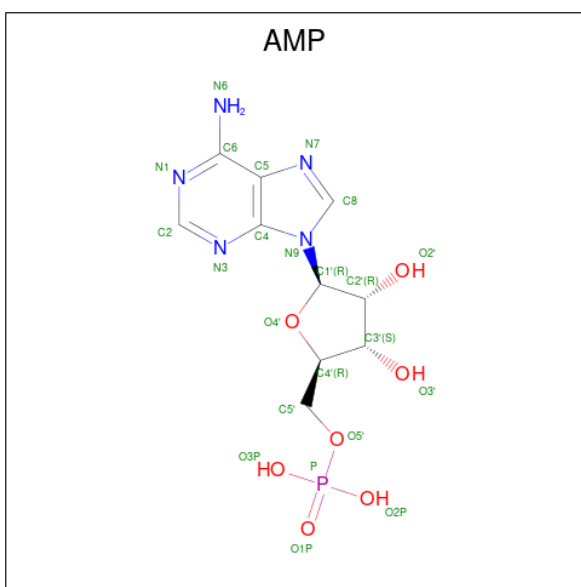
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP R4R1U5
A	-1	PRO	-	expression tag	UNP R4R1U5
A	0	ALA	-	expression tag	UNP R4R1U5
B	-2	GLY	-	expression tag	UNP R4R1U5
B	-1	PRO	-	expression tag	UNP R4R1U5
B	0	ALA	-	expression tag	UNP R4R1U5
C	-2	GLY	-	expression tag	UNP R4R1U5
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 (CCD ID: 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 (CCD ID: 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			

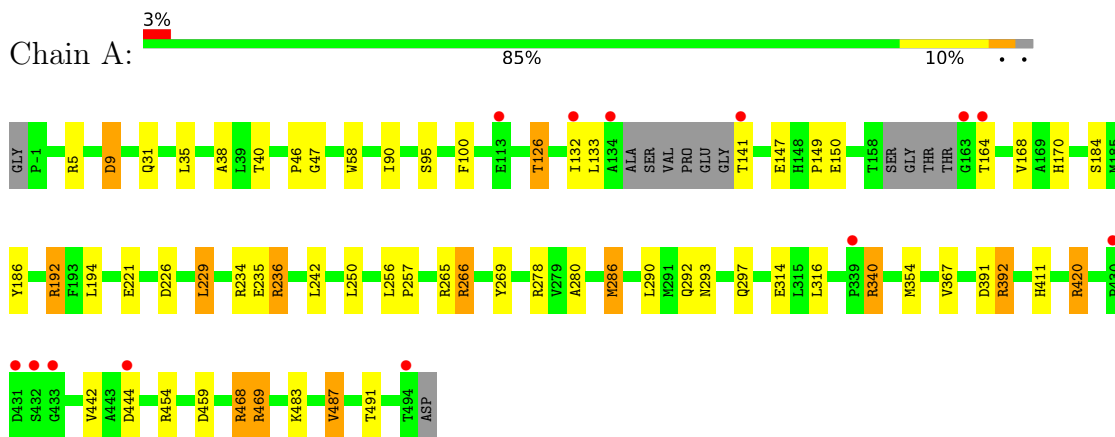
- Molecule 4 is water.

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		

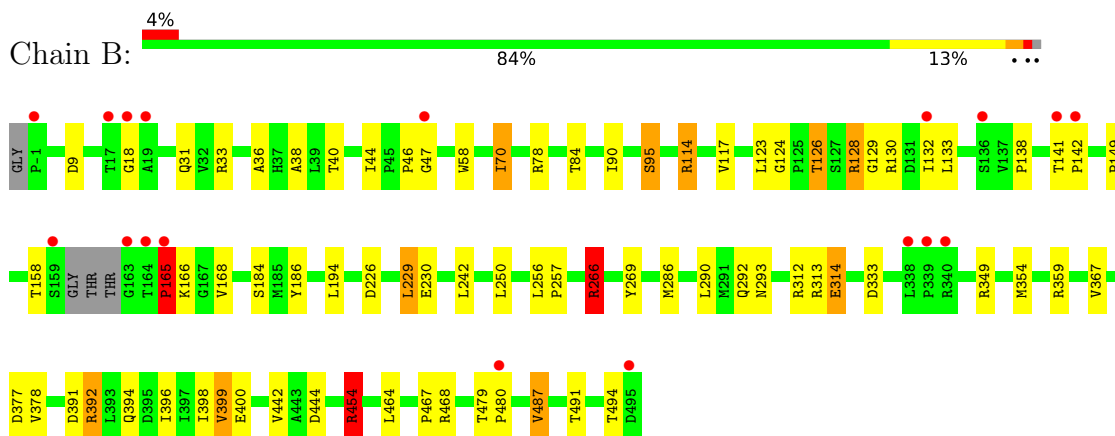
3 Residue-property plots [i](#)

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.

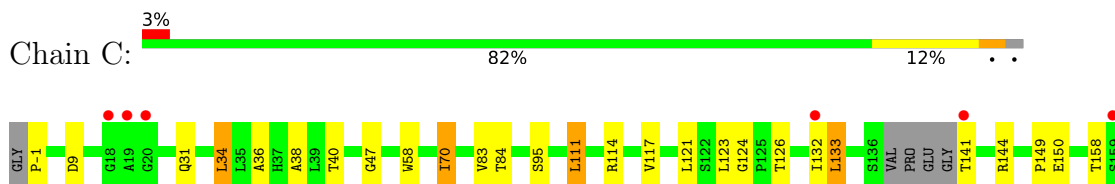
- Molecule 1: Fatty acid CoA ligase

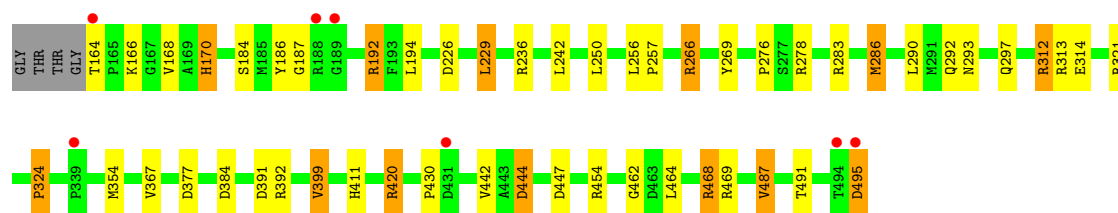


- Molecule 1: Fatty acid CoA ligase

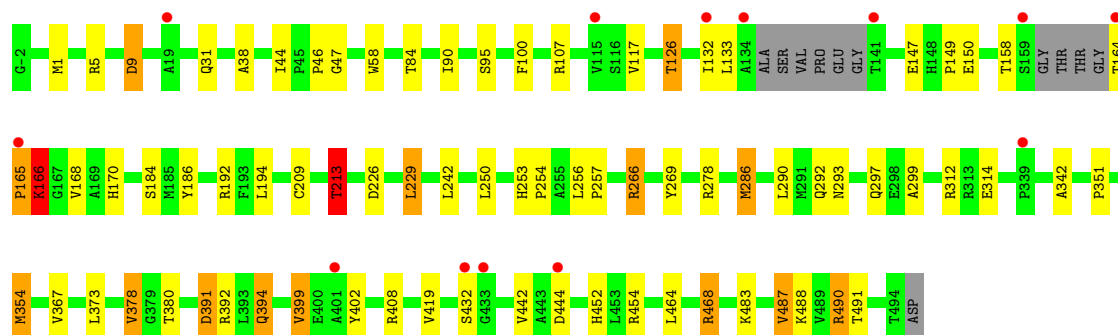
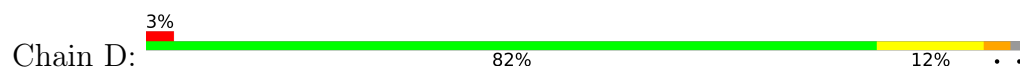


- Molecule 1: Fatty acid CoA ligase

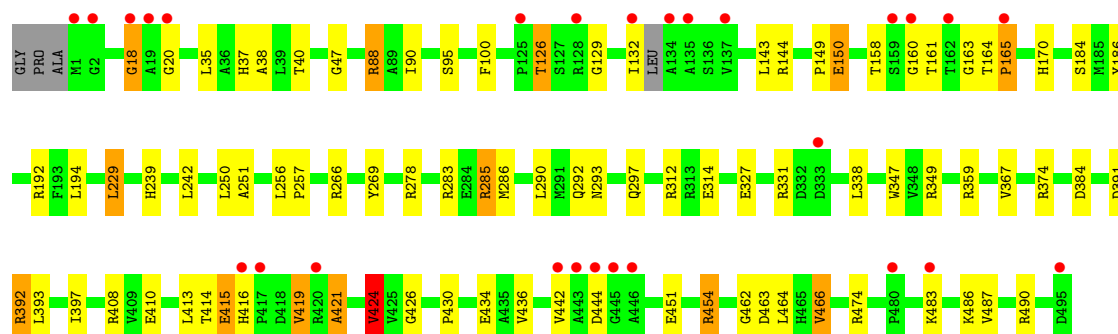
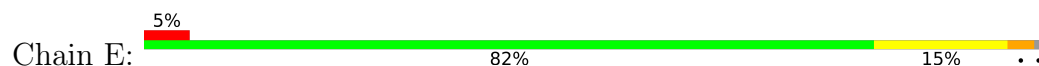




● Molecule 1: Fatty acid CoA ligase



● 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 , 46.4	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: EQ2, AMP

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	0.81	0/3660	1.03	0/5009
1	B	0.82	1/3717 (0.0%)	1.05	1/5089 (0.0%)
1	C	0.84	1/3702 (0.0%)	1.05	4/5065 (0.1%)
1	D	0.86	1/3664 (0.0%)	1.06	1/5014 (0.0%)
1	E	0.87	3/3676 (0.1%)	1.10	3/5038 (0.1%)
All	All	0.84	6/18419 (0.0%)	1.06	9/25215 (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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	129	GLY	N-CA	5.91	1.51	1.45
1	E	239	HIS	CE1-NE2	5.62	1.38	1.32
1	B	129	GLY	N-CA	5.43	1.51	1.45
1	C	170	HIS	CE1-NE2	5.37	1.38	1.32
1	D	351	PRO	C-O	-5.11	1.17	1.24
1	E	421	ALA	N-CA	5.02	1.52	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	THR	N-CA-CB	-7.44	99.48	110.49
1	C	187	GLY	CA-C-O	-6.06	118.09	122.45
1	B	165	PRO	N-CA-CB	-5.90	97.06	103.25
1	E	462	GLY	CA-C-O	-5.68	118.22	122.37
1	E	150	GLU	CB-CG-CD	5.62	122.15	112.60
1	C	462	GLY	CA-C-O	-5.35	117.36	122.13
1	E	424	VAL	N-CA-CB	5.31	118.47	111.25
1	C	324	PRO	N-CA-C	5.16	123.09	112.47
1	C	-1	PRO	N-CA-CB	5.04	108.54	103.00

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

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Mol	Chain	Res	Type	Group
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 ⓘ

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	36	0
1	B	3634	0	3574	38	0
1	C	3615	0	3558	41	0
1	D	3584	0	3525	38	0
1	E	3594	0	3513	35	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	5	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	183	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 (183) 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:D:168:VAL:HG13	1:D:354:MET:HE3	1.55	0.89
1:B:392:ARG:NH1	3:B:502:AMP:O3'	2.08	0.86
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:A:168:VAL:HG13	1:A:354:MET:HE3	1.62	0.80
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:C:168:VAL:HG13	1:C:354:MET:HE3	1.67	0.76
1:B:168:VAL:HG13	1:B:354:MET:HE3	1.67	0.76
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
1:B:377:ASP:CG	3:B:502:AMP:HO3'	2.01	0.68
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: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:B:392:ARG:HH11	3:B:502:AMP:HO3'	1.51	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:C:34:LEU:HD12	1:C:34:LEU:C	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:342:ALA:O	1:D:380:THR:OG1	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:E:143:LEU:HD23	1:E:143:LEU:C	2.39	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: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:D:90:ILE:O	1:D:95:SER:OG	2.31	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:C:34:LEU:C	1:C:34:LEU:CD1	2.91	0.44
1:E:38:ALA:CB	1:E:132:ILE:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:392:ARG:HH11	3:A:502:AMP:HO3'	1.63	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:E:90:ILE:O	1:E:95:SER:OG	2.33	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
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:D:250:LEU:HD23	1:D:286:MET:HE1	2.02	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:B:377:ASP:OD1	3:B:502:AMP:O3'	2.35	0.42
1:A:250:LEU:HD23	1:A:286:MET:HE1	2.01	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
1:C:123:LEU:C	1:C:133:LEU:HD22	2.45	0.42
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:250:LEU:HD23	1:C:286:MET:HE1	2.03	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:B:90:ILE:O	1:B:95:SER:OG	2.35	0.41
1:D:229:LEU:HD12	1:D:229:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:90:ILE:O	1:A:95:SER:OG	2.34	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

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	480/498 (96%)	468 (98%)	11 (2%)	1 (0%)	43	66
1	B	490/498 (98%)	476 (97%)	10 (2%)	4 (1%)	16	34
1	C	485/498 (97%)	470 (97%)	13 (3%)	2 (0%)	30	51
1	D	481/498 (97%)	465 (97%)	12 (2%)	4 (1%)	16	34
1	E	490/498 (98%)	473 (96%)	13 (3%)	4 (1%)	16	34
All	All	2426/2490 (97%)	2352 (97%)	59 (2%)	15 (1%)	21	42

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 ⓘ

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%)	330 (93%)	25 (7%)	14	31
1	B	362/384 (94%)	327 (90%)	35 (10%)	8	17
1	C	361/384 (94%)	327 (91%)	34 (9%)	8	18
1	D	356/384 (93%)	326 (92%)	30 (8%)	10	23
1	E	353/384 (92%)	325 (92%)	28 (8%)	11	26
All	All	1787/1920 (93%)	1635 (92%)	152 (8%)	10	22

All (152) 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

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Mol	Chain	Res	Type
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	236	ARG
1	A	278	ARG
1	A	286	MET
1	A	290	LEU
1	A	314	GLU
1	A	340	ARG
1	A	367	VAL
1	A	391	ASP
1	A	392	ARG
1	A	420	ARG
1	A	442	VAL
1	A	469	ARG
1	A	487	VAL
1	B	9	ASP
1	B	40	THR
1	B	46	PRO
1	B	70	ILE
1	B	84	THR
1	B	95	SER
1	B	114	ARG
1	B	117	VAL
1	B	123	LEU
1	B	126	THR
1	B	128	ARG
1	B	133	LEU
1	B	165	PRO
1	B	184	SER
1	B	194	LEU
1	B	226	ASP
1	B	229	LEU
1	B	230	GLU
1	B	266	ARG
1	B	286	MET

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Mol	Chain	Res	Type
1	B	290	LEU
1	B	313	ARG
1	B	314	GLU
1	B	333	ASP
1	B	367	VAL
1	B	391	ASP
1	B	392	ARG
1	B	394	GLN
1	B	398	ILE
1	B	399	VAL
1	B	400	GLU
1	B	442	VAL
1	B	454	ARG
1	B	487	VAL
1	B	494	THR
1	C	9	ASP
1	C	34	LEU
1	C	40	THR
1	C	70	ILE
1	C	84	THR
1	C	95	SER
1	C	111	LEU
1	C	117	VAL
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	194	LEU
1	C	226	ASP
1	C	229	LEU
1	C	286	MET
1	C	290	LEU
1	C	313	ARG
1	C	314	GLU
1	C	324	PRO
1	C	367	VAL
1	C	391	ASP

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Mol	Chain	Res	Type
1	C	399	VAL
1	C	420[A]	ARG
1	C	420[B]	ARG
1	C	442	VAL
1	C	444	ASP
1	C	487	VAL
1	C	495	ASP
1	D	9	ASP
1	D	46	PRO
1	D	84	THR
1	D	107	ARG
1	D	117	VAL
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	194	LEU
1	D	213	THR
1	D	226	ASP
1	D	229	LEU
1	D	266	ARG
1	D	278	ARG
1	D	286	MET
1	D	290	LEU
1	D	314	GLU
1	D	354	MET
1	D	367	VAL
1	D	378	VAL
1	D	391	ASP
1	D	394	GLN
1	D	399	VAL
1	D	442	VAL
1	D	487	VAL
1	D	488	LYS
1	D	490	ARG
1	E	40	THR
1	E	126	THR
1	E	150	GLU
1	E	161	THR
1	E	164	THR

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Mol	Chain	Res	Type
1	E	165	PRO
1	E	184	SER
1	E	194	LEU
1	E	229	LEU
1	E	286	MET
1	E	290	LEU
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	483	LYS
1	E	486	LYS
1	E	487	VAL
1	E	490	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	37	HIS
1	A	54	HIS
1	A	170	HIS
1	A	208	GLN
1	A	253	HIS
1	A	293	ASN
1	A	386	HIS
1	A	388	HIS
1	A	452	HIS
1	B	37	HIS
1	B	54	HIS
1	B	170	HIS
1	B	253	HIS
1	B	293	ASN

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Mol	Chain	Res	Type
1	B	386	HIS
1	B	388	HIS
1	B	394	GLN
1	B	465	HIS
1	C	37	HIS
1	C	54	HIS
1	C	170	HIS
1	C	253	HIS
1	C	293	ASN
1	C	386	HIS
1	C	388	HIS
1	C	465	HIS
1	D	54	HIS
1	D	170	HIS
1	D	208	GLN
1	D	249	GLN
1	D	253	HIS
1	D	293	ASN
1	D	297	GLN
1	D	386	HIS
1	D	388	HIS
1	D	394	GLN
1	D	452	HIS
1	D	465	HIS
1	E	54	HIS
1	E	208	GLN
1	E	245	ASN
1	E	253	HIS
1	E	293	ASN
1	E	386	HIS
1	E	388	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 [i](#)

There are no oligosaccharides 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
2	EQ2	A	501	-	20,21,21	0.60	0	29,31,31	0.97	1 (3%)
3	AMP	C	502	-	25,25,25	1.56	4 (16%)	37,38,38	1.98	8 (21%)
2	EQ2	E	501	-	20,21,21	0.89	1 (5%)	29,31,31	0.96	1 (3%)
2	EQ2	B	501	-	20,21,21	0.67	0	29,31,31	1.03	3 (10%)
2	EQ2	C	501	-	20,21,21	0.95	1 (5%)	29,31,31	1.17	3 (10%)
3	AMP	E	502	-	21,21,25	1.88	4 (19%)	31,31,38	2.25	10 (32%)
3	AMP	D	502	-	25,25,25	1.60	3 (12%)	37,38,38	1.99	9 (24%)
2	EQ2	D	501	-	20,21,21	0.54	0	29,31,31	1.00	1 (3%)
3	AMP	B	502	-	25,25,25	1.61	5 (20%)	37,38,38	1.96	10 (27%)
3	AMP	A	502	-	25,25,25	1.60	4 (16%)	37,38,38	1.91	12 (32%)

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	EQ2	A	501	-	-	4/8/8/8	0/3/3/3
3	AMP	C	502	-	-	0/10/26/26	0/3/3/3
2	EQ2	E	501	-	-	4/8/8/8	0/3/3/3
2	EQ2	B	501	-	-	8/8/8/8	0/3/3/3
2	EQ2	C	501	-	-	4/8/8/8	0/3/3/3
3	AMP	E	502	-	-	0/6/22/26	0/3/3/3

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

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	502	AMP	C5-C4	6.22	1.50	1.39
3	D	502	AMP	C5-C4	5.36	1.48	1.39
3	A	502	AMP	C5-C4	5.16	1.48	1.39
3	B	502	AMP	C5-C4	4.97	1.47	1.39
3	C	502	AMP	C5-C4	4.88	1.47	1.39
3	E	502	AMP	C8-N7	3.30	1.38	1.31
2	C	501	EQ2	C14-C3	3.03	1.44	1.40
3	D	502	AMP	C5-C6	2.87	1.49	1.41
3	C	502	AMP	C8-N7	2.86	1.37	1.31
3	C	502	AMP	C5-C6	2.82	1.48	1.41
3	A	502	AMP	C5-C6	2.82	1.48	1.41
3	E	502	AMP	C5-C6	2.72	1.48	1.41
3	B	502	AMP	C8-N7	2.66	1.36	1.31
3	A	502	AMP	C4-N9	-2.53	1.32	1.37
3	B	502	AMP	C5-N7	-2.52	1.34	1.39
3	A	502	AMP	C8-N7	2.51	1.36	1.31
3	D	502	AMP	C8-N7	2.39	1.36	1.31
3	B	502	AMP	C5-C6	2.31	1.47	1.41
3	B	502	AMP	C4-N9	-2.31	1.32	1.37
2	E	501	EQ2	C4-C5	2.09	1.54	1.50
3	E	502	AMP	C5-N7	-2.05	1.35	1.39
3	C	502	AMP	C4-N9	-2.00	1.33	1.37

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	502	AMP	C5-C4-N3	-6.37	117.94	126.72
3	D	502	AMP	C5-C4-N3	-5.83	118.70	126.72
3	C	502	AMP	C5-C4-N3	-5.44	119.22	126.72
3	B	502	AMP	C5-C4-N3	-5.38	119.31	126.72
3	D	502	AMP	N3-C4-N9	5.19	136.00	127.17
3	E	502	AMP	N3-C4-N9	4.84	135.40	127.17
3	A	502	AMP	C5-C4-N3	-4.50	120.52	126.72
3	C	502	AMP	N3-C4-N9	4.48	134.79	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	AMP	N3-C2-N1	-4.37	121.97	128.58
3	C	502	AMP	C2-N3-C4	4.33	122.41	111.83
3	D	502	AMP	N3-C2-N1	-4.23	122.19	128.58
3	B	502	AMP	N3-C4-N9	4.21	134.33	127.17
3	D	502	AMP	C2-N3-C4	4.14	121.95	111.83
3	B	502	AMP	C2-N3-C4	3.76	121.02	111.83
3	E	502	AMP	C2-N3-C4	3.74	120.96	111.83
3	A	502	AMP	N3-C4-N9	3.73	133.52	127.17
3	B	502	AMP	N3-C2-N1	-3.72	122.94	128.58
3	A	502	AMP	C4-N9-C8	3.65	109.57	105.74
3	A	502	AMP	C4-C5-N7	-3.40	106.69	110.58
3	E	502	AMP	C2'-C1'-N9	-3.36	104.95	113.30
3	E	502	AMP	N3-C2-N1	-3.32	123.56	128.58
3	B	502	AMP	O4'-C1'-N9	3.27	114.37	108.09
3	E	502	AMP	O4'-C1'-N9	3.22	114.28	108.09
2	C	501	EQ2	C3-C14-N2	3.10	133.81	130.76
3	A	502	AMP	C2-N3-C4	2.91	118.94	111.83
3	E	502	AMP	C3'-C2'-C1'	2.89	106.93	101.46
3	E	502	AMP	C4-C5-N7	-2.84	107.34	110.58
2	A	501	EQ2	O3-C5-C4	-2.82	115.62	121.30
3	C	502	AMP	C4-N9-C8	2.79	108.67	105.74
3	B	502	AMP	O4'-C4'-C5'	2.79	118.26	109.33
3	A	502	AMP	N3-C2-N1	-2.70	124.49	128.58
3	C	502	AMP	C6-C5-N7	2.54	136.98	132.09
3	D	502	AMP	C4-N9-C8	2.53	108.39	105.74
3	A	502	AMP	C2'-C3'-C4'	2.46	107.36	102.61
3	A	502	AMP	C5-N7-C8	2.45	107.30	103.45
3	C	502	AMP	C4-C5-N7	-2.45	107.79	110.58
3	A	502	AMP	N9-C8-N7	-2.44	110.47	113.94
2	C	501	EQ2	C7-C14-C3	-2.33	118.39	120.10
3	B	502	AMP	O4'-C4'-C3'	-2.33	100.53	105.15
3	A	502	AMP	C6-C5-N7	2.31	136.54	132.09
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	D	502	AMP	C4-C5-N7	-2.24	108.02	110.58
3	D	502	AMP	N6-C6-N1	2.24	123.37	118.38
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	E	501	EQ2	C3-N1-C4	2.17	120.86	118.01
2	D	501	EQ2	O3-C5-C4	-2.15	116.96	121.30
3	A	502	AMP	O4'-C1'-N9	2.12	112.16	108.09
2	B	501	EQ2	C3-C14-N2	2.11	132.84	130.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	502	AMP	C4-C5-N7	-2.09	108.19	110.58
3	E	502	AMP	C2-N1-C6	2.09	122.16	118.73
2	B	501	EQ2	C3-N1-C4	2.05	120.70	118.01
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	D	502	AMP	C5-C6-N6	-2.02	118.29	123.29
3	C	502	AMP	O2P-P-O1P	2.01	118.69	110.83
3	D	502	AMP	C2-N1-C6	2.00	122.02	118.73

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

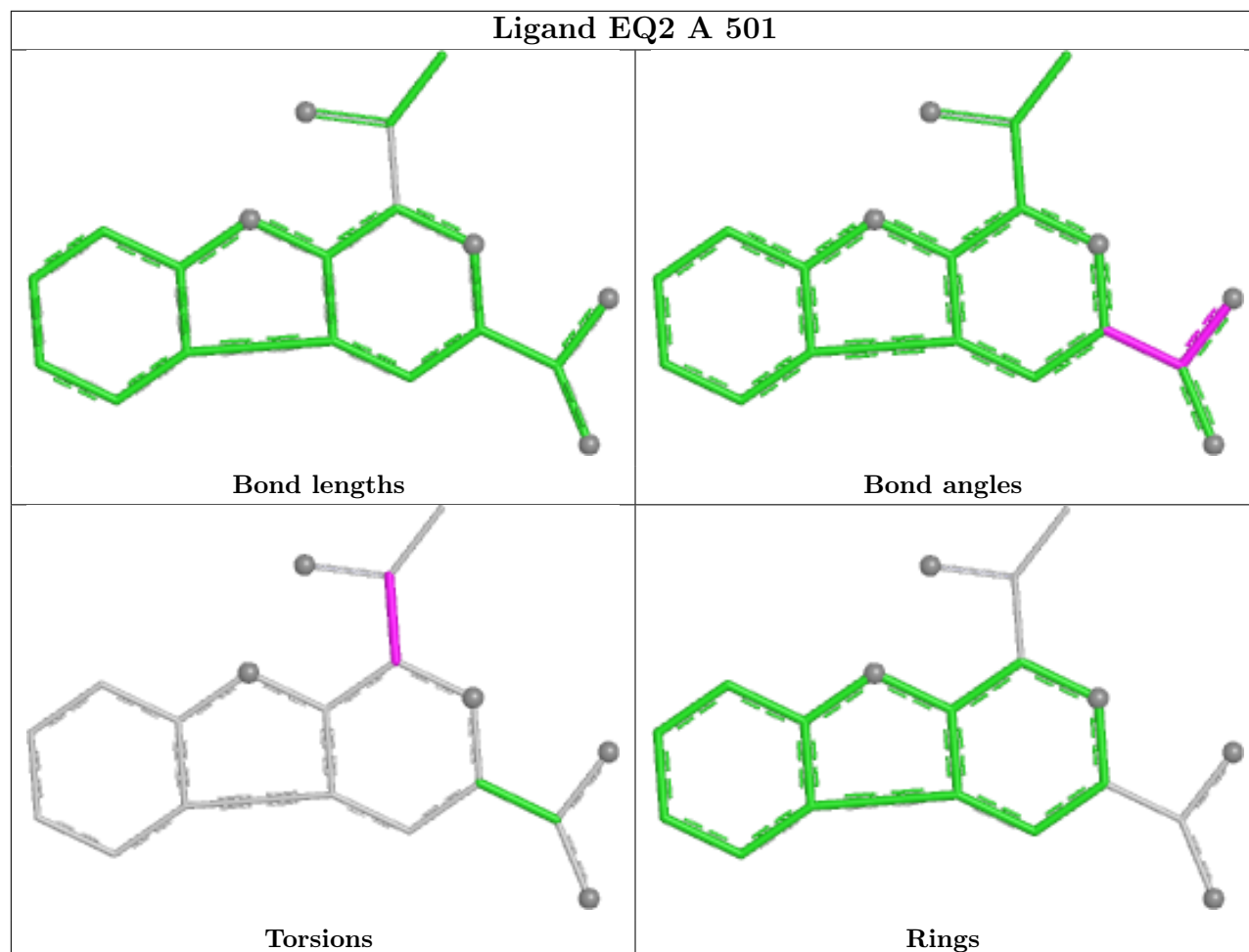
There are no ring outliers.

5 monomers are involved in 18 short contacts:

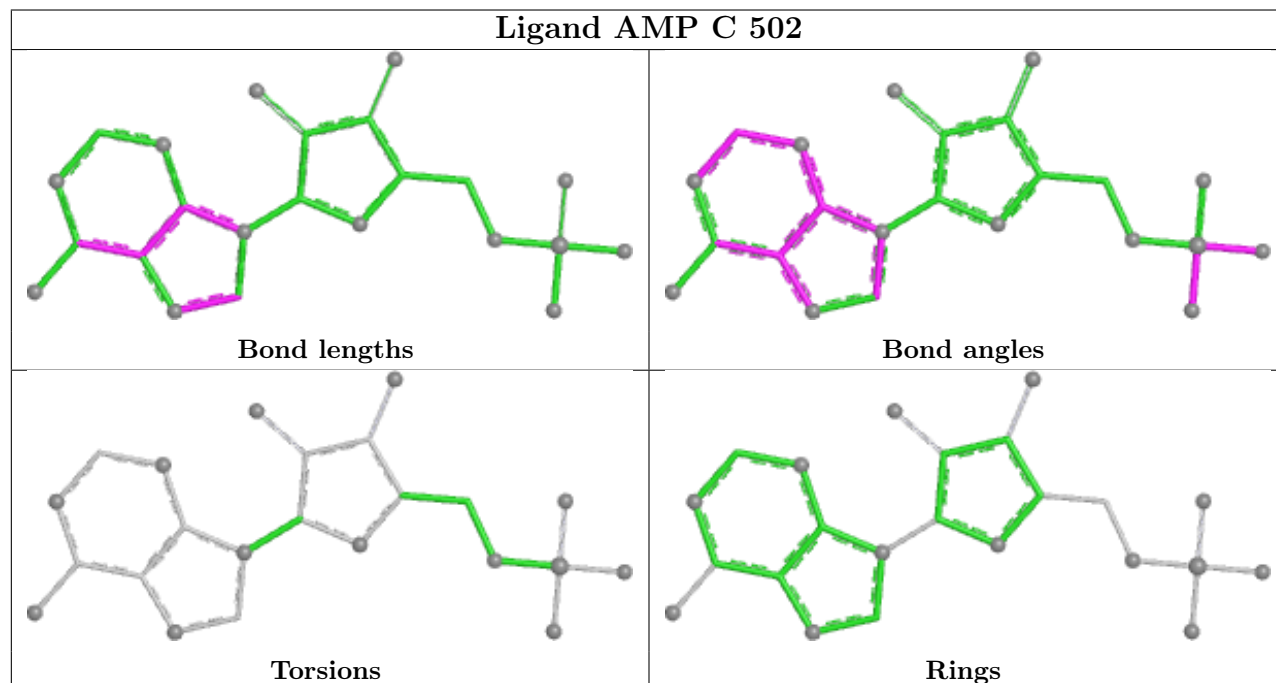
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	AMP	3	0
2	C	501	EQ2	2	0
3	D	502	AMP	4	0
3	B	502	AMP	5	0
3	A	502	AMP	5	0

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.

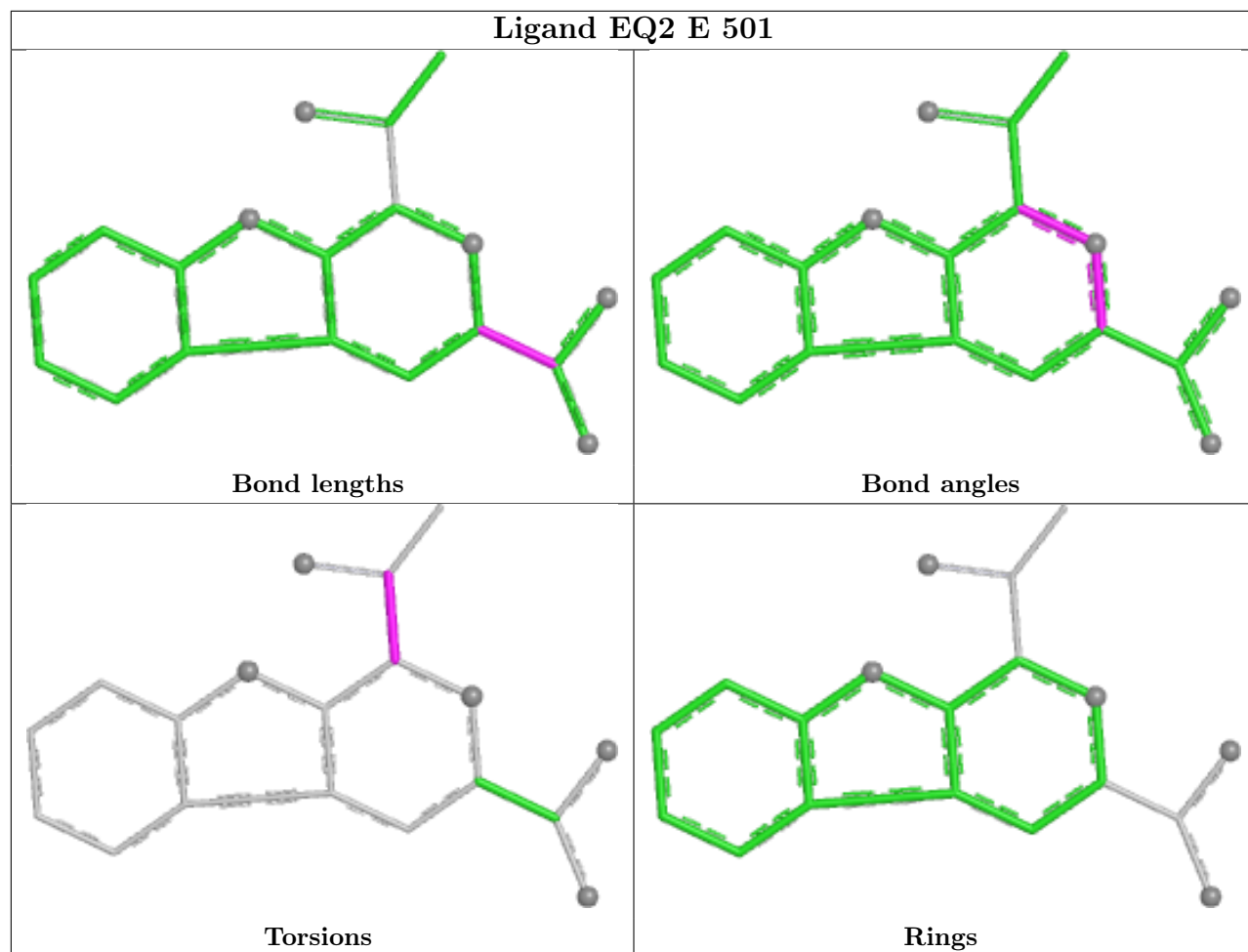
Ligand EQ2 A 501



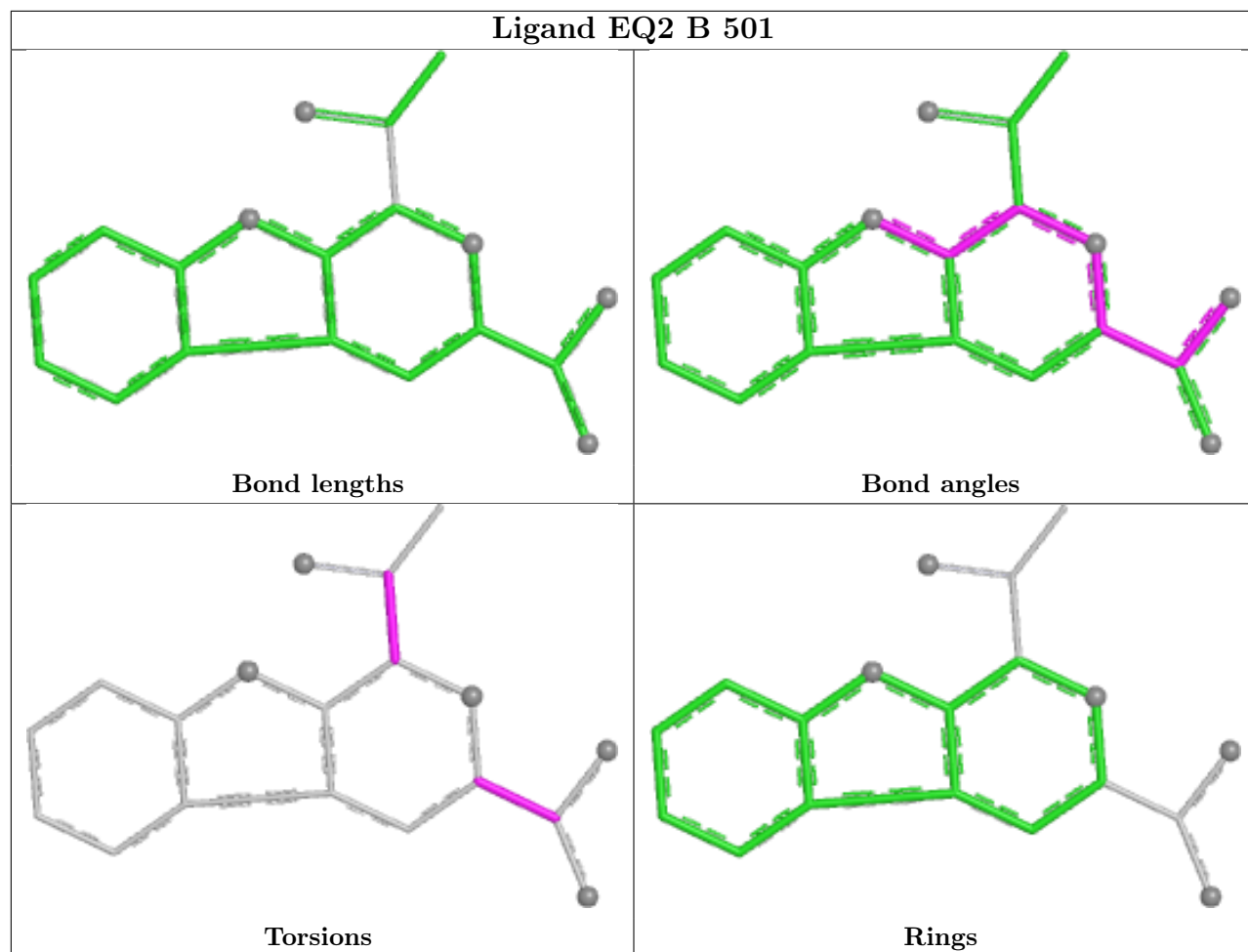
Ligand AMP C 502



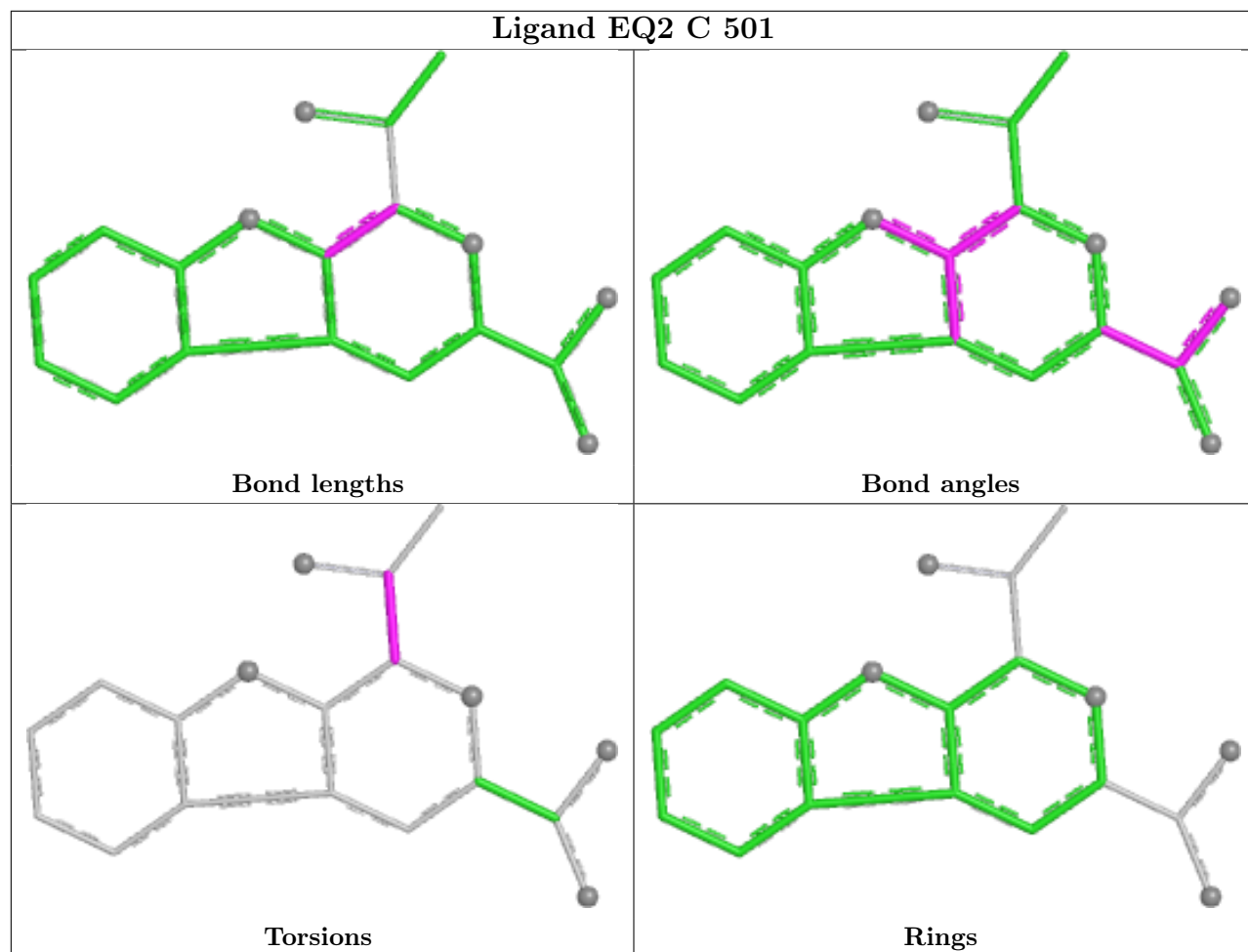
Ligand EQ2 E 501



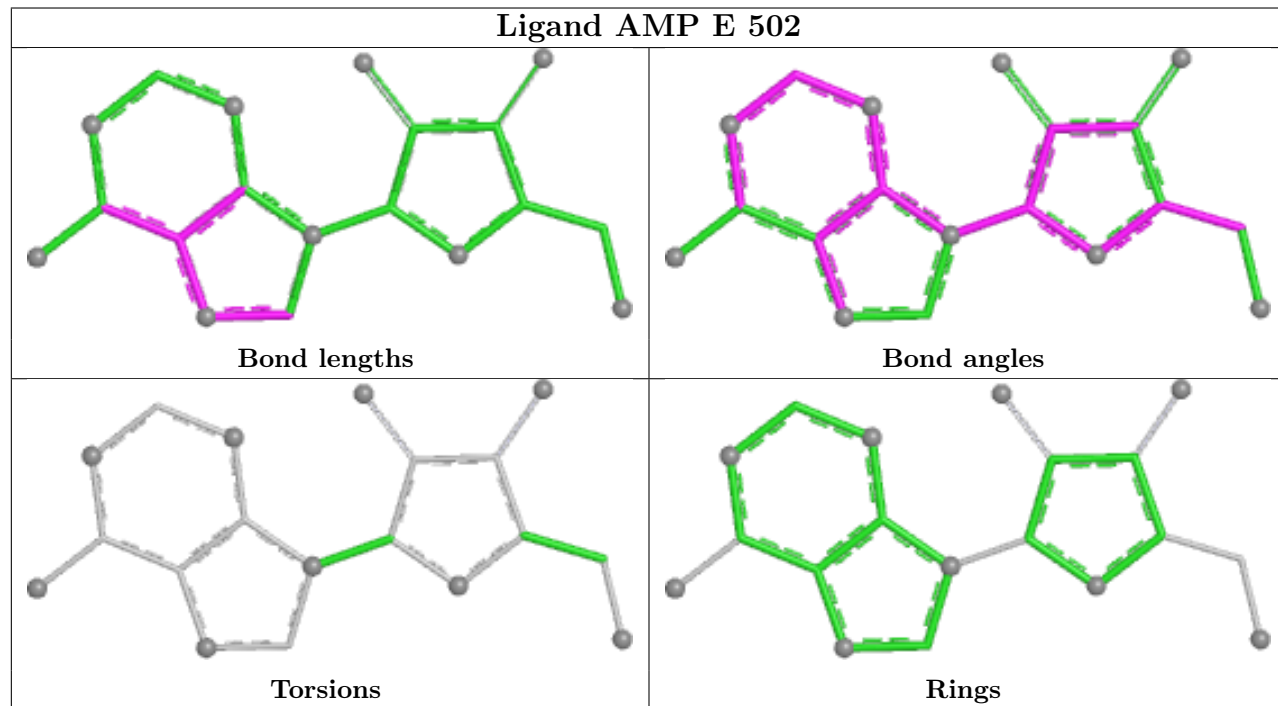
Ligand EQ2 B 501



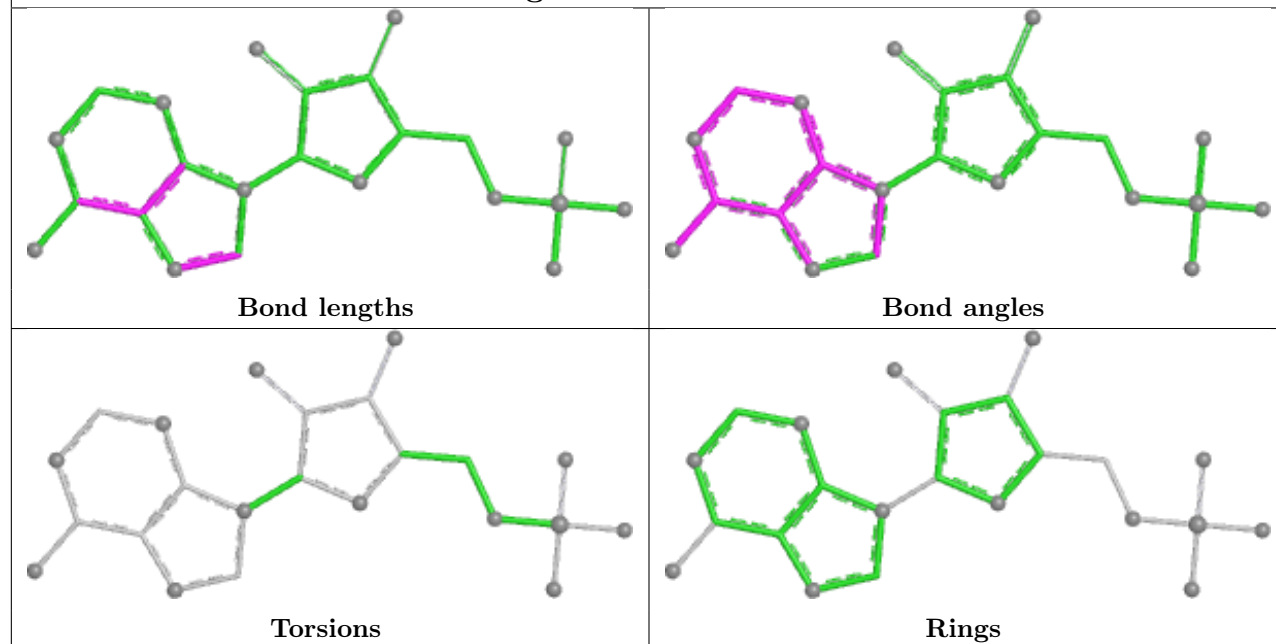
Ligand EQ2 C 501



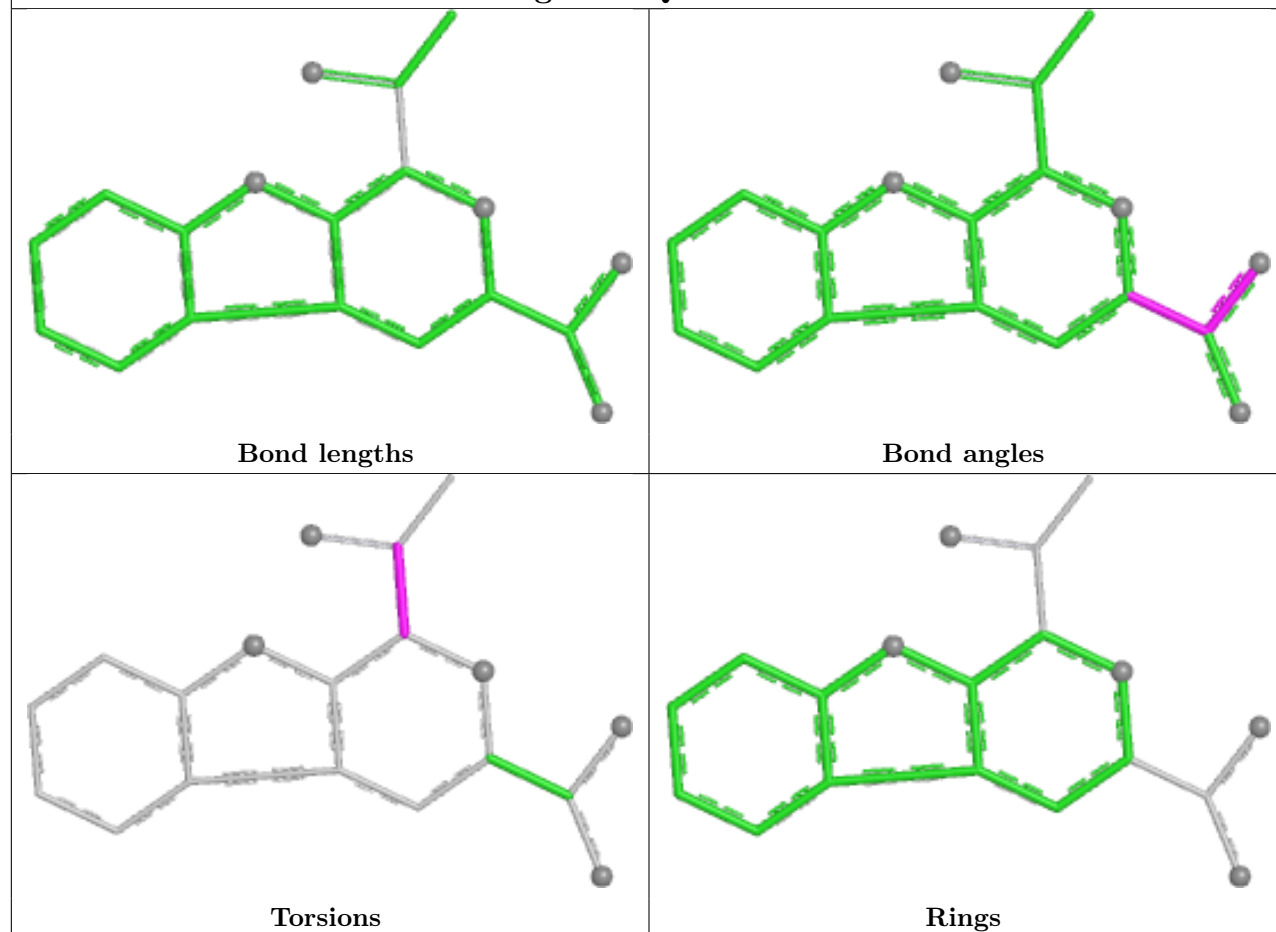
Ligand AMP E 502

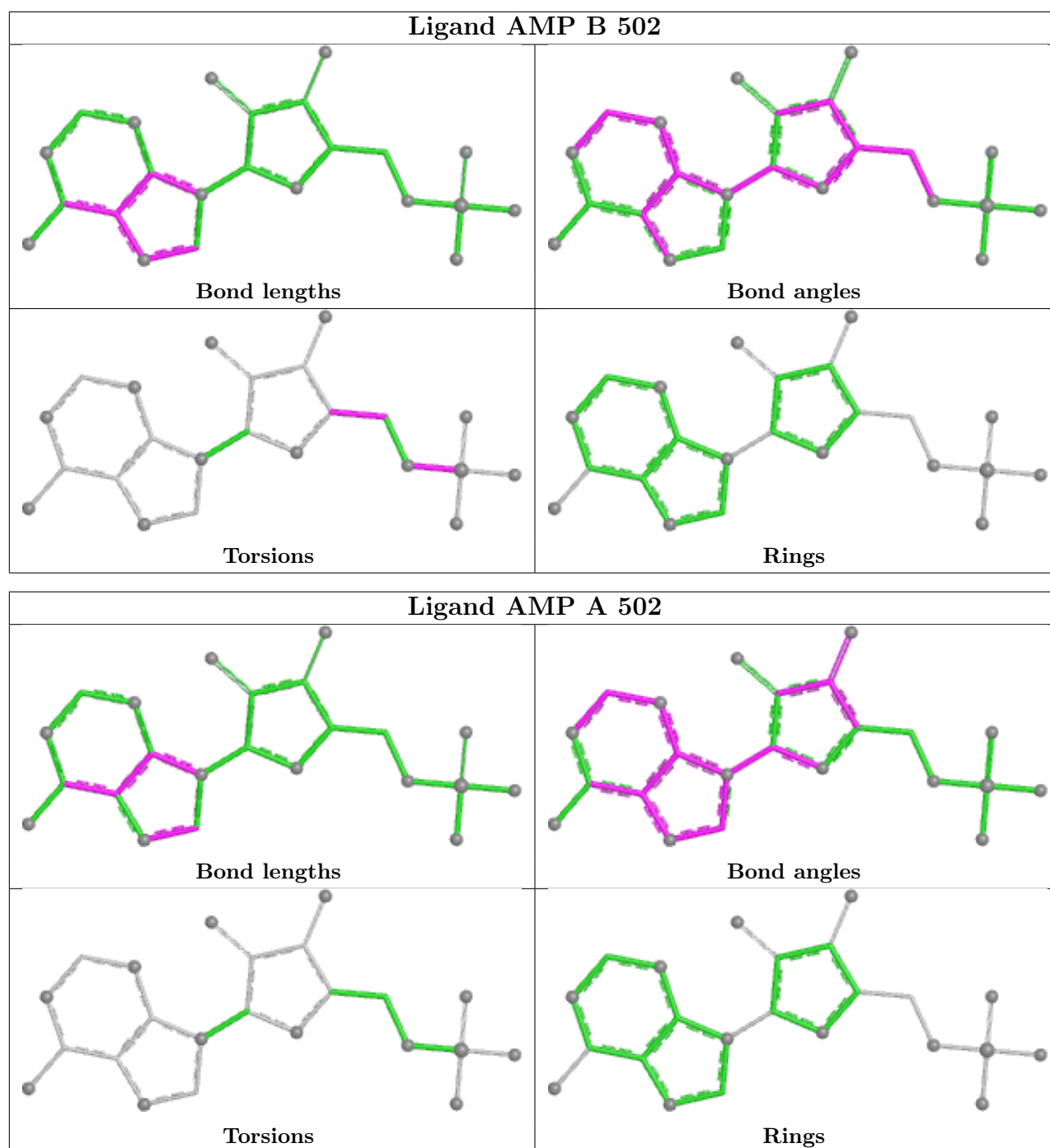


Ligand AMP D 502



Ligand EQ2 D 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	13 (2%) 56 50	17, 36, 63, 95	0
1	B	494/498 (99%)	0.12	18 (3%) 46 40	19, 36, 64, 104	0
1	C	489/498 (98%)	0.09	13 (2%) 56 50	13, 35, 63, 91	2 (0%)
1	D	487/498 (97%)	0.17	13 (2%) 56 50	21, 37, 69, 90	0
1	E	494/498 (99%)	0.45	27 (5%) 30 25	27, 46, 77, 111	0
All	All	2450/2490 (98%)	0.19	84 (3%) 48 42	13, 39, 68, 111	2 (0%)

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	SER	5.4
1	E	19	ALA	4.7
1	E	134	ALA	4.5
1	B	159	SER	4.5
1	E	1	MET	4.2
1	B	495	ASP	4.1
1	A	134	ALA	3.9
1	E	159	SER	3.9
1	D	165	PRO	3.8
1	E	446	ALA	3.7
1	A	433	GLY	3.7
1	B	165	PRO	3.6
1	C	159	SER	3.5
1	D	159	SER	3.5
1	E	445	GLY	3.5
1	B	163	GLY	3.4
1	C	188	ARG	3.4
1	A	141	THR	3.3
1	E	444	ASP	3.3
1	C	494	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	164	THR	3.2
1	E	160	GLY	3.1
1	C	19	ALA	3.1
1	C	339	PRO	3.0
1	C	20	GLY	3.0
1	E	20	GLY	2.9
1	D	19	ALA	2.9
1	C	495	ASP	2.9
1	C	431	ASP	2.9
1	D	432	SER	2.8
1	D	444	ASP	2.8
1	A	113	GLU	2.8
1	D	433	GLY	2.8
1	E	18	GLY	2.8
1	A	132	ILE	2.8
1	B	19	ALA	2.8
1	B	-1	PRO	2.8
1	D	339	PRO	2.8
1	E	443	ALA	2.8
1	E	132	ILE	2.7
1	B	136	SER	2.7
1	E	480	PRO	2.7
1	B	340	ARG	2.6
1	B	47	GLY	2.6
1	A	339	PRO	2.6
1	B	132	ILE	2.6
1	D	164	THR	2.6
1	C	141	THR	2.5
1	B	17	THR	2.5
1	C	164	THR	2.5
1	B	339	PRO	2.5
1	B	18	GLY	2.5
1	E	420	ARG	2.4
1	A	494	THR	2.4
1	D	134	ALA	2.4
1	D	141	THR	2.4
1	C	18	GLY	2.4
1	E	128	ARG	2.4
1	E	162	THR	2.4
1	A	164	THR	2.3
1	E	135	ALA	2.3
1	E	416	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	480	PRO	2.3
1	D	401	ALA	2.3
1	A	431	ASP	2.3
1	A	444	ASP	2.3
1	A	163	GLY	2.2
1	B	338	LEU	2.2
1	D	115	VAL	2.2
1	E	442	VAL	2.2
1	C	132	ILE	2.2
1	E	333	ASP	2.2
1	E	125	PRO	2.2
1	C	189	GLY	2.1
1	E	495	ASP	2.1
1	E	137	VAL	2.1
1	A	430	PRO	2.1
1	E	2	GLY	2.1
1	E	483	LYS	2.1
1	D	132	ILE	2.1
1	B	142	PRO	2.0
1	E	165	PRO	2.0
1	B	141	THR	2.0
1	E	417	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

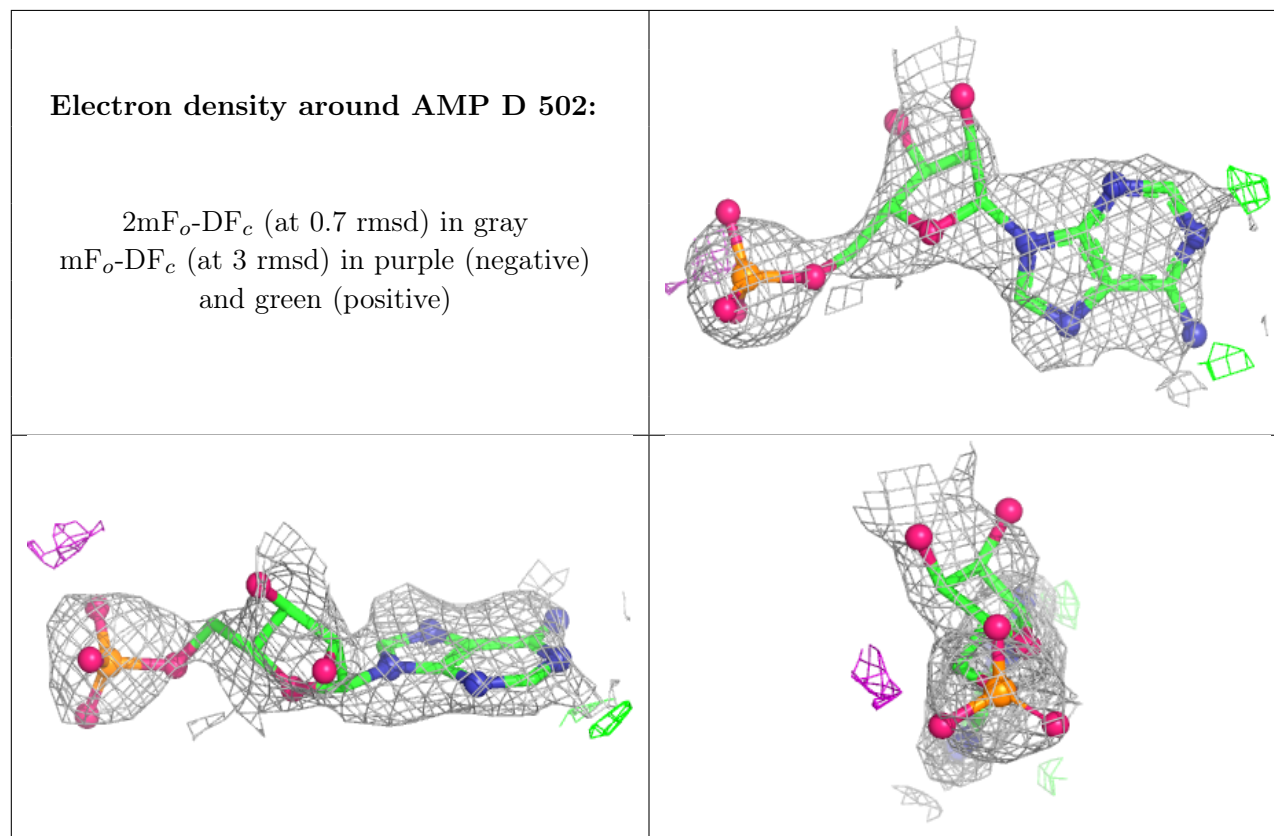
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	AMP	D	502	23/23	0.84	0.16	82,93,103,105	0

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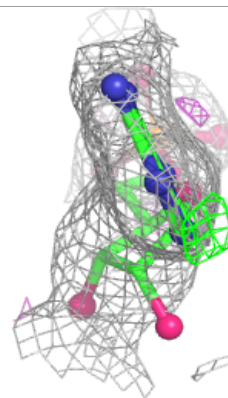
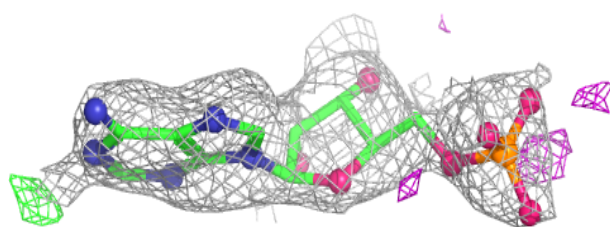
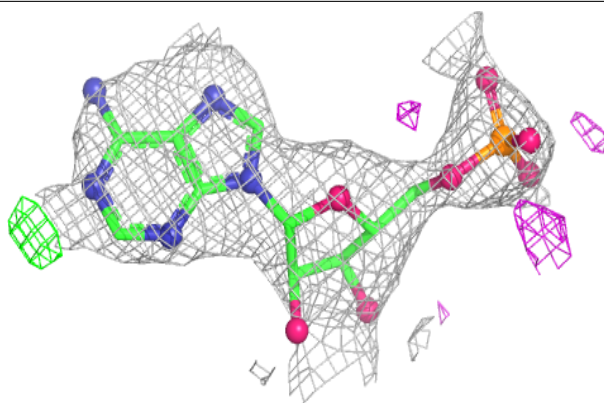
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	AMP	C	502	23/23	0.86	0.15	67,78,104,106	0
3	AMP	B	502	23/23	0.87	0.13	52,64,105,108	0
3	AMP	A	502	23/23	0.89	0.13	59,69,81,88	0
2	EQ2	E	501	19/19	0.92	0.12	41,55,61,63	0
3	AMP	E	502	19/23	0.92	0.10	47,52,55,55	0
2	EQ2	A	501	19/19	0.95	0.07	34,37,45,45	0
2	EQ2	B	501	19/19	0.95	0.08	35,39,49,51	0
2	EQ2	D	501	19/19	0.95	0.08	36,38,43,43	0
2	EQ2	C	501	19/19	0.96	0.07	33,36,42,44	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.

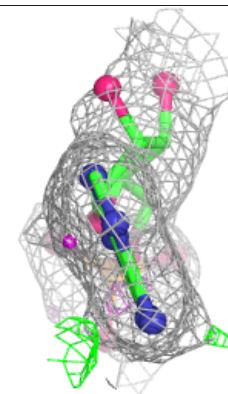
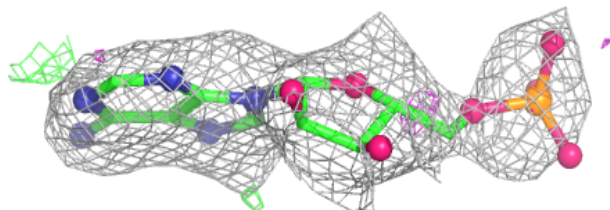
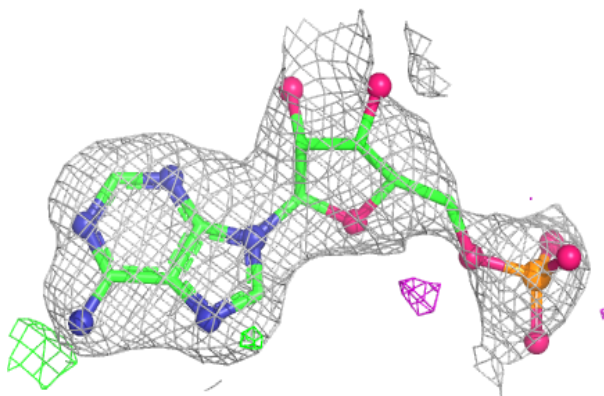


Electron density around AMP C 502:

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

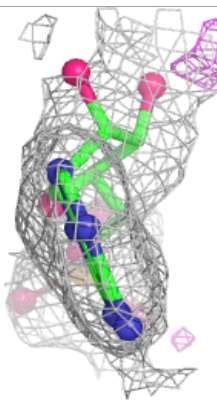
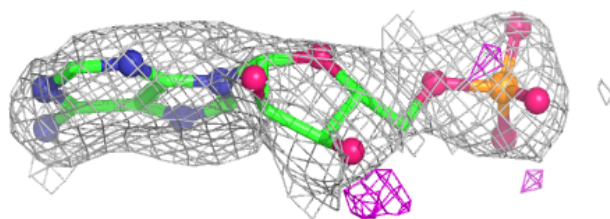
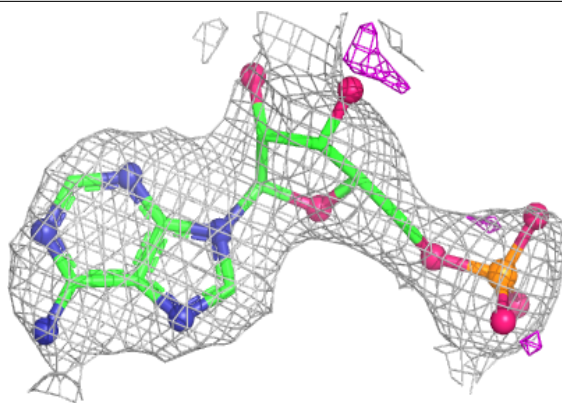
**Electron density around AMP B 502:**

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



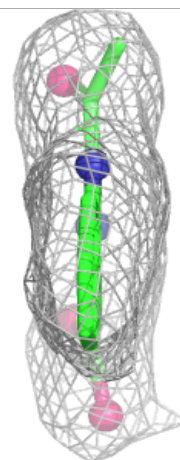
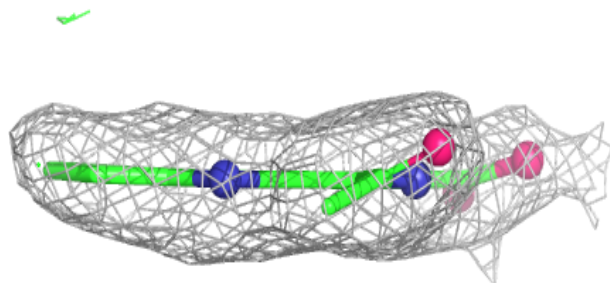
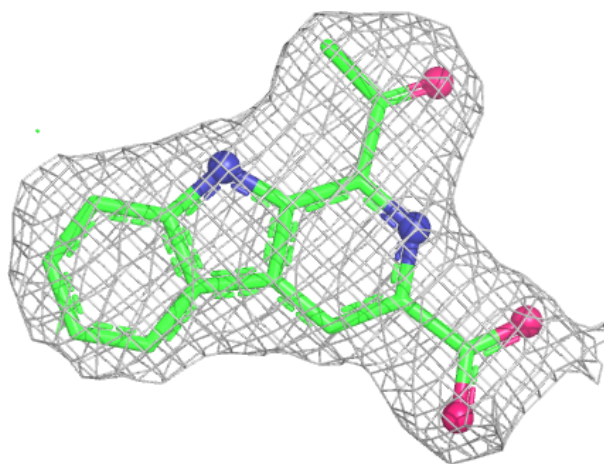
Electron density around AMP A 502:

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



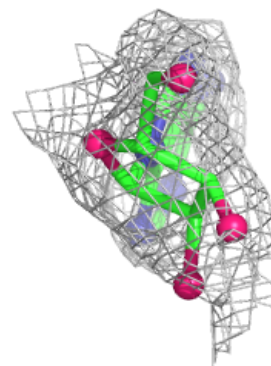
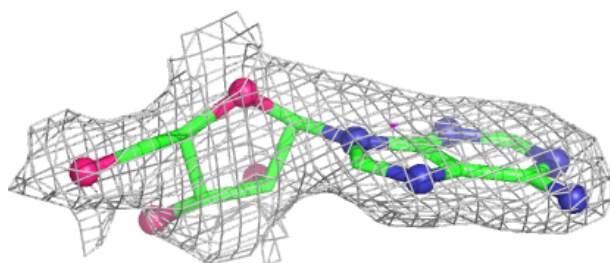
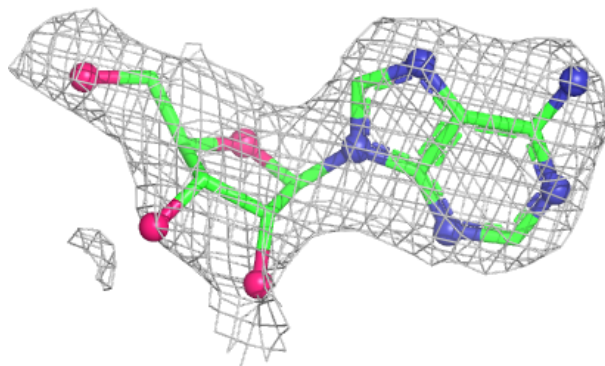
Electron density around EQ2 E 501:

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



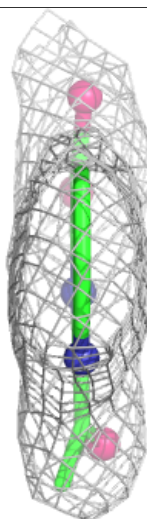
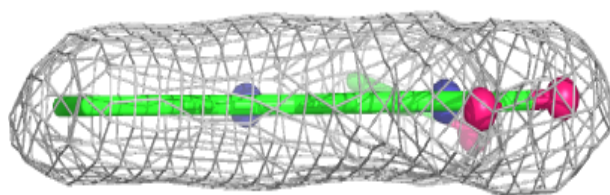
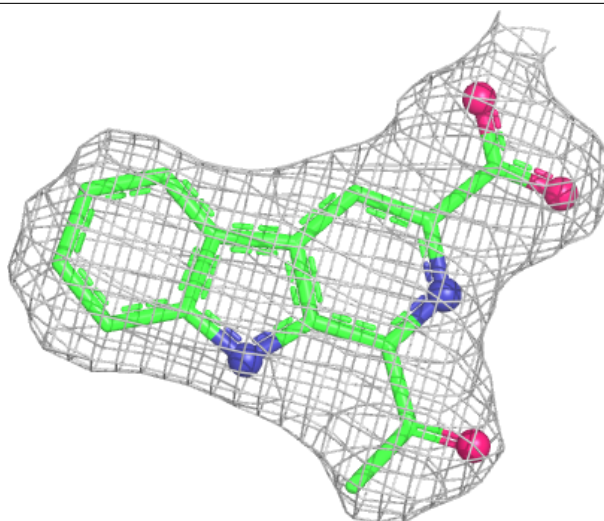
Electron density around AMP E 502:

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



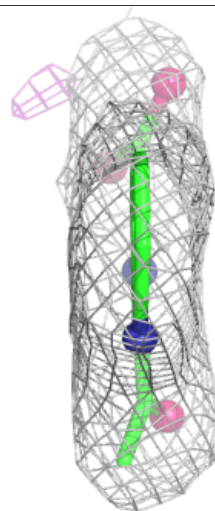
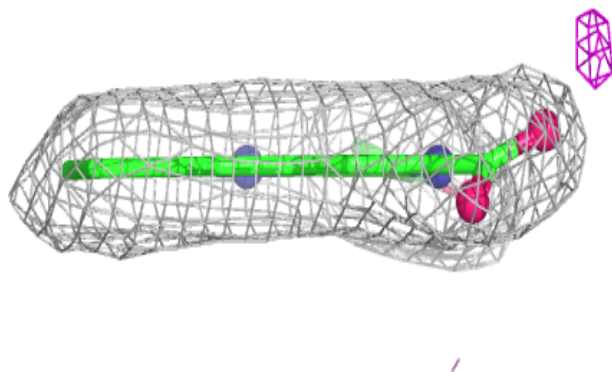
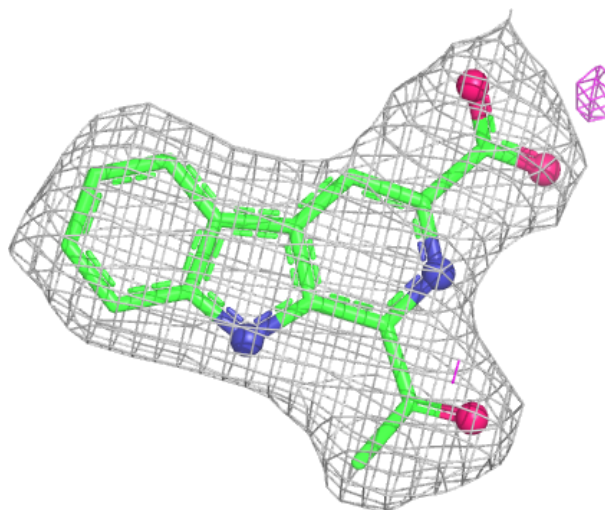
Electron density around EQ2 A 501:

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



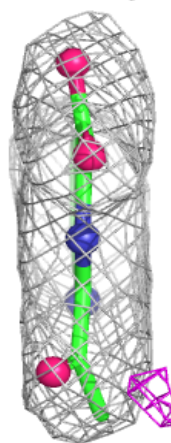
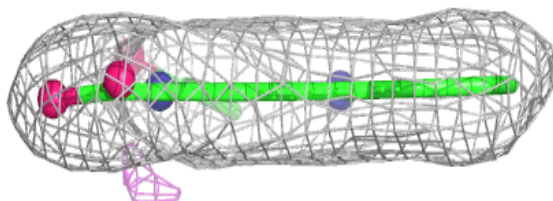
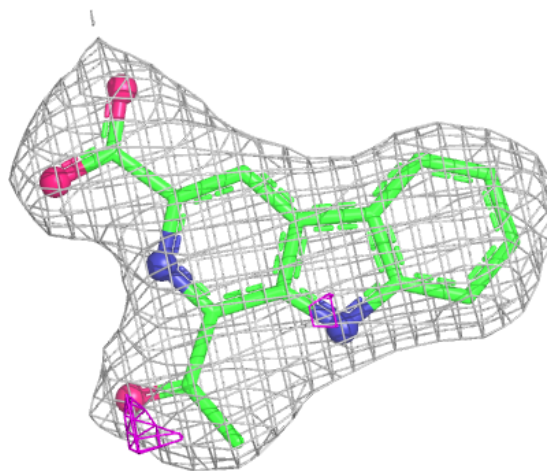
Electron density around EQ2 B 501:

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



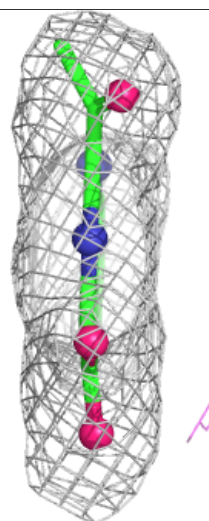
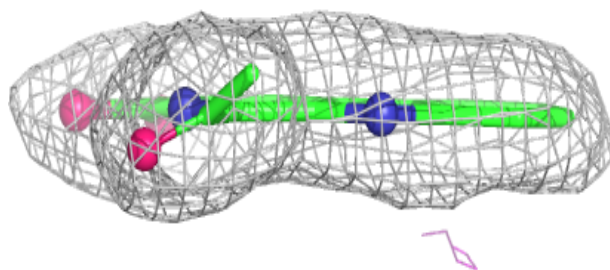
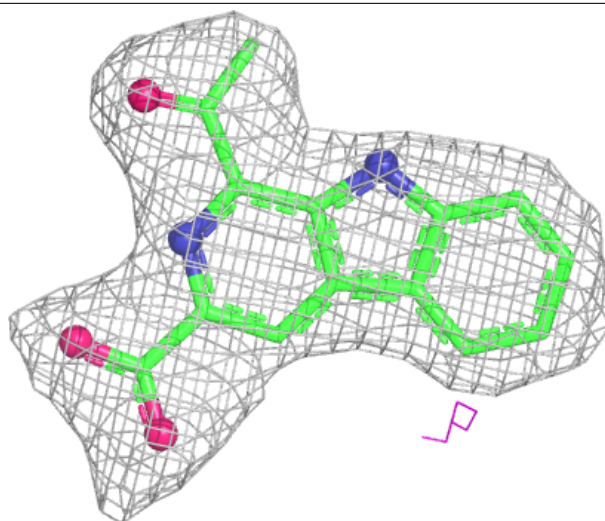
Electron density around EQ2 D 501:

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.