



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:40 pm BST

PDB ID : 6O2Y
Title : Crystal structure of IDH1 R132H mutant in complex with compound 24
Authors : Toms, A.V.; Lin, J.
Deposited on : 2019-02-25
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

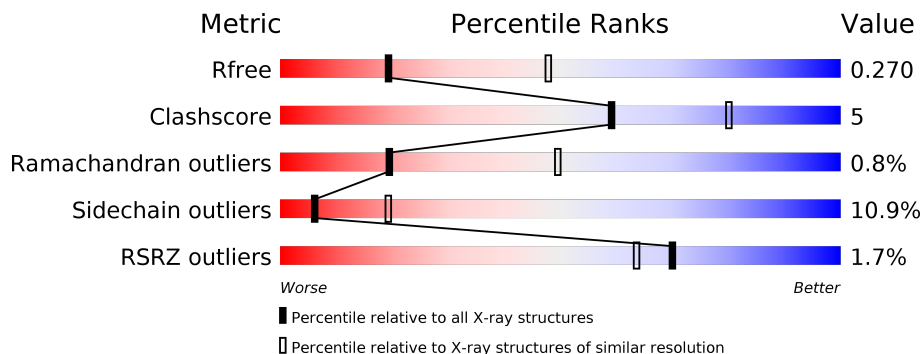
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 on 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	425	 82% 14% . .
1	B	425	 76% 20% . .
1	C	425	 5% 73% 21% . .

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 9978 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	413	3274	2082	554	620	18	0	0	0
1	B	411	3252	2068	550	616	18	0	0	0
1	C	409	3209	2041	541	609	18	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

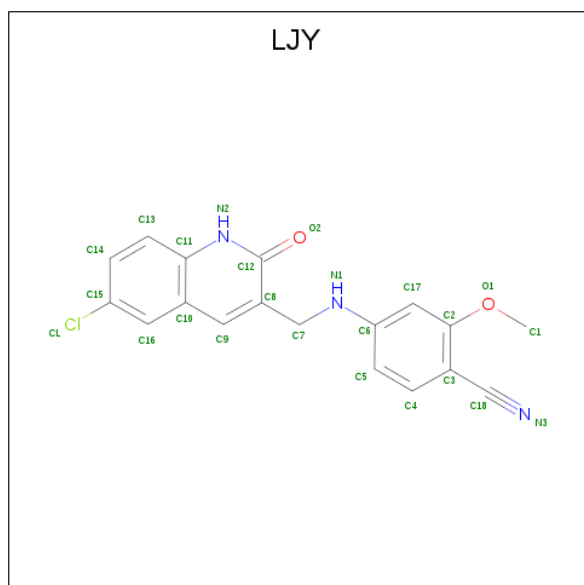
Chain	Residue	Modelled	Actual	Comment	Reference
A	132	HIS	ARG	engineered mutation	UNP O75874
A	415	GLU	-	expression tag	UNP O75874
A	416	LEU	-	expression tag	UNP O75874
A	417	GLU	-	expression tag	UNP O75874
A	418	HIS	-	expression tag	UNP O75874
A	419	HIS	-	expression tag	UNP O75874
A	420	HIS	-	expression tag	UNP O75874
A	421	HIS	-	expression tag	UNP O75874
A	422	HIS	-	expression tag	UNP O75874
A	423	HIS	-	expression tag	UNP O75874
A	424	HIS	-	expression tag	UNP O75874
A	425	HIS	-	expression tag	UNP O75874
B	132	HIS	ARG	engineered mutation	UNP O75874
B	415	GLU	-	expression tag	UNP O75874
B	416	LEU	-	expression tag	UNP O75874
B	417	GLU	-	expression tag	UNP O75874
B	418	HIS	-	expression tag	UNP O75874
B	419	HIS	-	expression tag	UNP O75874
B	420	HIS	-	expression tag	UNP O75874
B	421	HIS	-	expression tag	UNP O75874
B	422	HIS	-	expression tag	UNP O75874
B	423	HIS	-	expression tag	UNP O75874
B	424	HIS	-	expression tag	UNP O75874

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Chain	Residue	Modelled	Actual	Comment	Reference
B	425	HIS	-	expression tag	UNP O75874
C	132	HIS	ARG	engineered mutation	UNP O75874
C	415	GLU	-	expression tag	UNP O75874
C	416	LEU	-	expression tag	UNP O75874
C	417	GLU	-	expression tag	UNP O75874
C	418	HIS	-	expression tag	UNP O75874
C	419	HIS	-	expression tag	UNP O75874
C	420	HIS	-	expression tag	UNP O75874
C	421	HIS	-	expression tag	UNP O75874
C	422	HIS	-	expression tag	UNP O75874
C	423	HIS	-	expression tag	UNP O75874
C	424	HIS	-	expression tag	UNP O75874
C	425	HIS	-	expression tag	UNP O75874

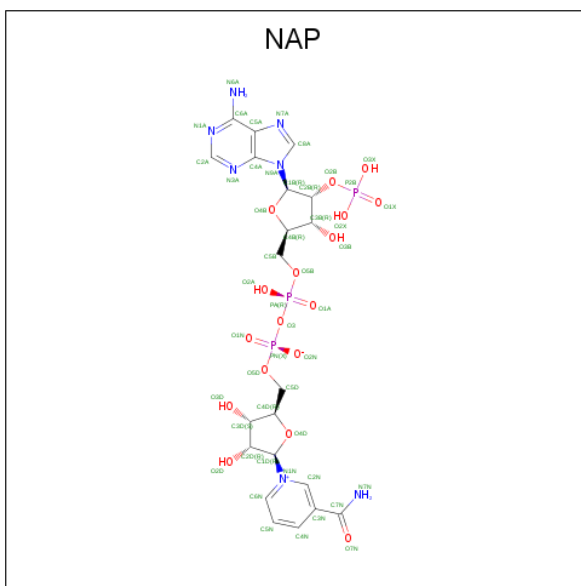
- Molecule 2 is 4-[[6-chloro-2-oxo-1,2-dihydroquinolin-3-yl)methyl]amino}-2-methoxybenzonitrile (three-letter code: LJY) (formula: C₁₈H₁₄ClN₃O₂) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Cl	N			O
2	A	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
2	B	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		
2	C	1	Total	C	Cl	N	O	0	0
			24	18	1	3	2		

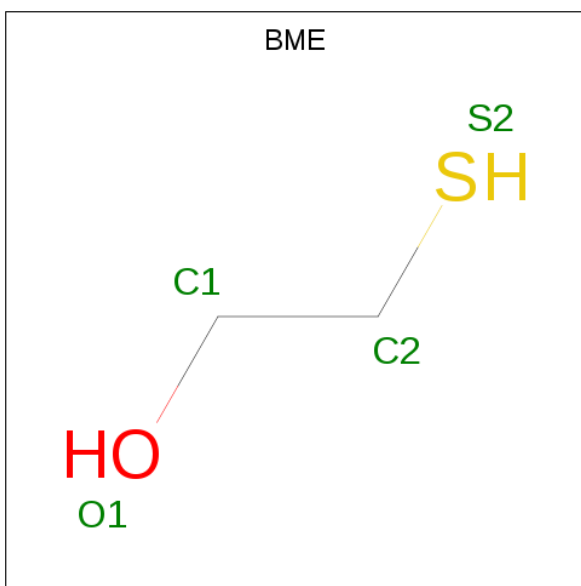
- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE

(three-letter code: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf		
			Total	C	N	O			P	
3	A	1	Total	48	21	7	17	3	0	0
3	B	1	Total	48	21	7	17	3	0	0
3	C	1	Total	48	21	7	17	3	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

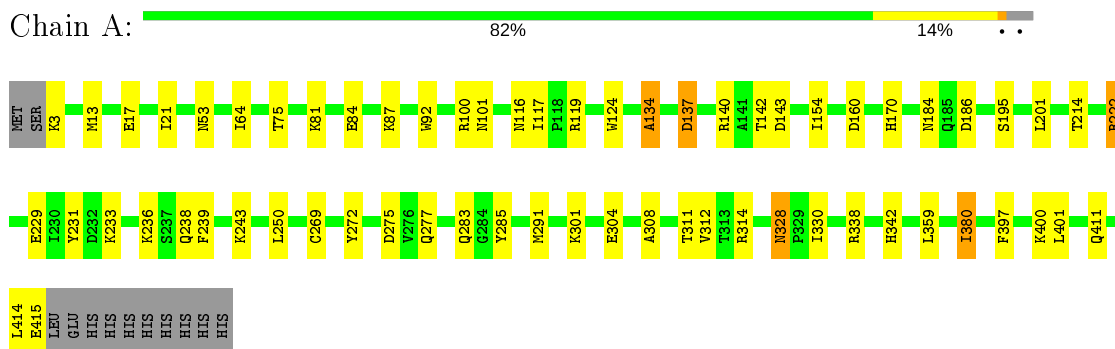
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	12	Total	O	0	0
			12	12		
5	B	8	Total	O	0	0
			8	8		
5	C	3	Total	O	0	0
			3	3		

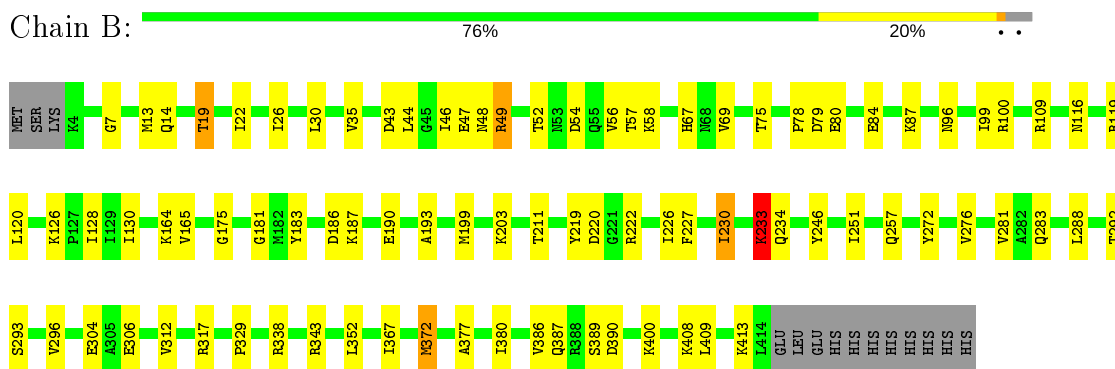
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

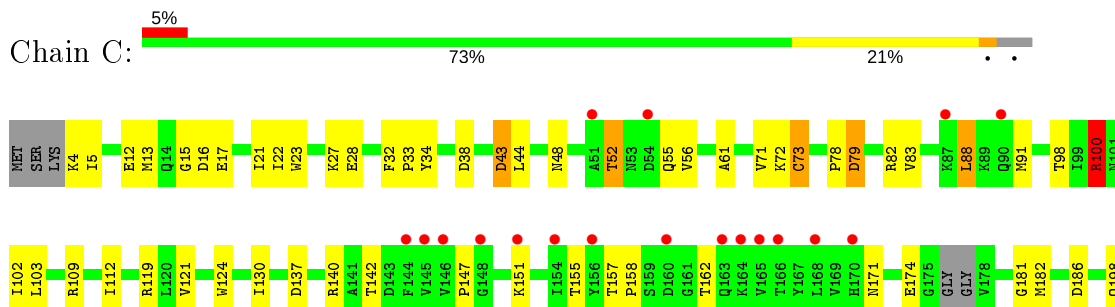
- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

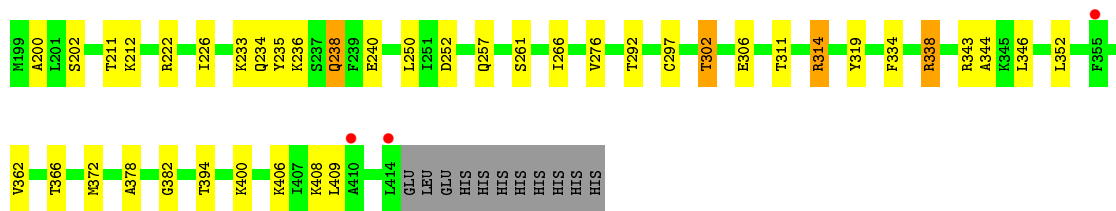


- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic



- Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	165.68Å 63.50Å 143.60Å 90.00° 99.52° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 44.16 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.80) 98.4 (44.16-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.81Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.209 , 0.275 0.208 , 0.270	Depositor DCC
R_{free} test set	1803 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	61.2	Xtrriage
Anisotropy	0.723	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9978	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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: LJY, NAP, BME

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	0.56	0/3343	0.73	0/4508
1	B	0.58	0/3321	0.78	1/4481 (0.0%)
1	C	0.61	0/3276	0.80	5/4426 (0.1%)
All	All	0.58	0/9940	0.77	6/13415 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	338	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	C	100	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	C	314	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	C	314	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	276	VAL	CB-CA-C	-5.06	101.79	111.40

There are no chirality outliers.

There are no planarity outliers.

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	3274	0	3239	29	0
1	B	3252	0	3209	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3209	0	3132	37	0
2	A	24	0	0	0	0
2	B	24	0	0	1	0
2	C	24	0	0	0	0
3	A	48	0	25	1	0
3	B	48	0	25	0	0
3	C	48	0	25	0	0
4	A	4	0	6	1	0
5	A	12	0	0	0	0
5	B	8	0	0	0	0
5	C	3	0	0	0	0
All	All	9978	0	9661	93	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 (93) 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:344:ALA:HB2	1:C:352:LEU:HD22	1.48	0.94
1:B:26:ILE:HG23	1:B:30:LEU:HD12	1.57	0.84
1:C:344:ALA:HB2	1:C:352:LEU:CD2	2.09	0.81
1:C:21:ILE:HG12	1:C:319:TYR:CE2	2.29	0.68
1:C:362:VAL:O	1:C:366:THR:HG23	1.93	0.68
1:C:61:ALA:HB1	1:C:102:ILE:HD11	1.78	0.66
1:C:83:VAL:HA	1:C:88:LEU:HD12	1.81	0.62
1:C:52:THR:HG22	1:C:55:GLN:HB3	1.81	0.61
1:B:199:MET:CE	1:B:296:VAL:HG21	2.31	0.60
1:B:22:ILE:O	1:B:26:ILE:HG13	2.03	0.58
1:A:53:ASN:HA	1:A:92:TRP:CH2	2.39	0.57
1:B:67:HIS:O	1:B:343:ARG:NH1	2.37	0.57
1:B:52:THR:OG1	1:B:56:VAL:HG12	2.05	0.56
1:C:43:ASP:OD1	1:C:43:ASP:O	2.24	0.55
1:B:199:MET:HE2	1:B:296:VAL:HG21	1.89	0.54
1:C:186:ASP:OD2	1:C:222:ARG:NH1	2.41	0.54
1:A:116:ASN:O	1:A:380:ILE:HD11	2.08	0.53
1:C:23:TRP:CE3	1:C:73:CYS:HB2	2.44	0.53
1:C:15:GLY:HA3	1:C:73:CYS:SG	2.49	0.53
1:A:13:MET:CE	1:A:64:ILE:HD11	2.40	0.52
1:B:109:ARG:NE	2:B:500:LJY:O2	2.41	0.52
1:C:378:ALA:O	1:C:382:GLY:N	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ALA:HB3	1:A:140:ARG:NH2	2.26	0.51
1:A:201:LEU:HD21	1:A:239:PHE:CD1	2.45	0.51
1:C:52:THR:HG21	1:C:56:VAL:HG23	1.91	0.51
1:A:275:ASP:HB3	1:A:277:GLN:OE1	2.12	0.50
1:C:130:ILE:N	1:C:130:ILE:HD12	2.26	0.50
1:C:212:LYS:NZ	1:C:252:ASP:OD1	2.45	0.50
1:A:117:ILE:HD13	1:A:380:ILE:HD11	1.95	0.49
1:C:17:GLU:HB2	1:C:311:THR:HB	1.95	0.49
1:A:214:THR:HG23	1:A:250:LEU:HD11	1.95	0.48
1:C:34:TYR:CD2	1:C:409:LEU:HD12	2.49	0.48
1:A:119:ARG:NE	1:A:124:TRP:O	2.45	0.48
1:B:43:ASP:HB3	1:B:48:ASN:ND2	2.28	0.48
1:B:128:ILE:HG22	1:B:130:ILE:CD1	2.44	0.48
1:C:43:ASP:OD1	1:C:48:ASN:HB3	2.15	0.47
1:B:120:LEU:HD12	1:B:281:VAL:HG13	1.96	0.47
1:C:297:CYS:HG	1:C:302:THR:HG1	1.62	0.47
1:A:75:THR:O	3:A:501:NAP:H2N	2.15	0.46
1:C:100:ARG:HG3	1:C:100:ARG:NH2	2.31	0.46
1:B:372:MET:CE	1:B:380:ILE:HD12	2.47	0.45
1:A:137:ASP:OD1	1:A:184:ASN:ND2	2.47	0.45
1:C:121:VAL:HG21	1:C:124:TRP:CZ2	2.52	0.45
1:A:13:MET:HE2	1:A:64:ILE:HD11	1.98	0.45
1:C:200:ALA:HA	1:C:266:ILE:HD12	1.99	0.45
1:C:79:ASP:O	1:C:82:ARG:N	2.50	0.45
1:A:17:GLU:HB2	1:A:311:THR:HB	1.99	0.45
1:A:269:CYS:SG	4:A:502:BME:S2	3.11	0.44
1:A:186:ASP:OD2	1:A:222:ARG:NH1	2.51	0.44
1:B:49:ARG:NH2	1:B:75:THR:HB	2.31	0.44
1:C:13:MET:HB3	1:C:44:LEU:CD1	2.48	0.44
1:B:116:ASN:ND2	1:B:367:ILE:O	2.49	0.44
1:C:13:MET:HB2	1:C:72:LYS:HA	1.99	0.44
1:A:154:ILE:HD11	1:B:181:GLY:HA3	2.00	0.44
1:B:19:THR:HA	1:B:22:ILE:HG22	1.98	0.44
1:A:186:ASP:OD1	1:A:222:ARG:NH1	2.51	0.44
1:C:16:ASP:HB3	1:C:17:GLU:HG3	1.99	0.44
1:A:291:MET:HB3	1:A:308:ALA:HB3	2.00	0.44
1:B:211:THR:HB	1:B:220:ASP:HB3	2.00	0.44
1:B:226:ILE:O	1:B:230:ILE:HG13	2.18	0.44
1:A:301:LYS:O	1:A:342:HIS:NE2	2.44	0.43
1:B:186:ASP:OD1	1:B:222:ARG:NH1	2.52	0.43
1:C:236:LYS:O	1:C:240:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:ALA:CB	1:C:102:ILE:HD11	2.46	0.43
1:C:13:MET:HB3	1:C:44:LEU:HD13	1.99	0.43
1:B:69:VAL:HG21	1:B:343:ARG:HB2	2.01	0.43
1:C:43:ASP:OD1	1:C:43:ASP:C	2.57	0.43
1:A:328:ASN:HD22	1:A:330:ILE:H	1.66	0.43
1:A:143:ASP:HB2	1:B:219:TYR:HB2	2.01	0.43
1:B:372:MET:CE	1:B:377:ALA:HA	2.48	0.43
1:B:44:LEU:HD21	1:B:57:THR:HA	2.01	0.42
1:C:235:TYR:HA	1:C:238:GLN:HE21	1.85	0.42
1:C:344:ALA:CB	1:C:352:LEU:HD22	2.34	0.42
1:B:193:ALA:HA	1:B:227:PHE:CZ	2.55	0.42
1:C:100:ARG:HH21	1:C:100:ARG:HG3	1.82	0.42
1:A:214:THR:HG23	1:A:250:LEU:CD1	2.50	0.42
1:B:233:LYS:HD2	1:B:234:GLN:HG2	2.01	0.42
1:A:142:THR:HG22	1:A:142:THR:O	2.20	0.41
1:A:231:TYR:CE2	1:A:236:LYS:HG3	2.55	0.41
1:B:283:GLN:HE22	1:B:288:LEU:HD11	1.85	0.41
1:B:96:ASN:ND2	1:B:306:GLU:OE2	2.54	0.41
1:B:246:TYR:C	1:B:246:TYR:CD2	2.92	0.41
1:C:22:ILE:HD11	1:C:394:THR:HG23	2.03	0.41
1:A:272:TYR:CD2	1:B:272:TYR:CD1	3.09	0.41
1:C:292:THR:HG21	1:C:334:PHE:CB	2.50	0.41
1:A:170:HIS:HB2	1:B:183:TYR:CD2	2.56	0.40
1:B:387:GLN:N	1:B:390:ASP:OD2	2.50	0.40
1:A:229:GLU:O	1:A:233:LYS:HB2	2.22	0.40
1:C:13:MET:HB2	1:C:71:VAL:O	2.22	0.40
1:A:137:ASP:HA	1:A:140:ARG:NH1	2.36	0.40
1:B:7:GLY:HA2	1:B:352:LEU:HD22	2.04	0.40
1:C:32:PHE:N	1:C:33:PRO:CD	2.84	0.40
1:A:397:PHE:CE2	1:A:401:LEU:HD11	2.56	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	411/425 (97%)	385 (94%)	24 (6%)	2 (0%)	29	61
1	B	409/425 (96%)	379 (93%)	26 (6%)	4 (1%)	15	44
1	C	405/425 (95%)	351 (87%)	50 (12%)	4 (1%)	15	44
All	All	1225/1275 (96%)	1115 (91%)	100 (8%)	10 (1%)	19	49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	414	LEU
1	B	54	ASP
1	B	175	GLY
1	B	78	PRO
1	B	233	LYS
1	C	147	PRO
1	C	78	PRO
1	A	134	ALA
1	C	158	PRO
1	C	181	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	349/361 (97%)	324 (93%)	25 (7%)	14	38
1	B	346/361 (96%)	307 (89%)	39 (11%)	6	18
1	C	337/361 (93%)	289 (86%)	48 (14%)	3	10
All	All	1032/1083 (95%)	920 (89%)	112 (11%)	6	19

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS

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Mol	Chain	Res	Type
1	A	21	ILE
1	A	81	LYS
1	A	84	GLU
1	A	87	LYS
1	A	100	ARG
1	A	101	ASN
1	A	137	ASP
1	A	160	ASP
1	A	195	SER
1	A	222	ARG
1	A	238	GLN
1	A	243	LYS
1	A	283	GLN
1	A	285	TYR
1	A	304	GLU
1	A	312	VAL
1	A	314	ARG
1	A	328	ASN
1	A	338	ARG
1	A	359	LEU
1	A	380	ILE
1	A	400	LYS
1	A	411	GLN
1	A	415	GLU
1	B	13	MET
1	B	14	GLN
1	B	19	THR
1	B	35	VAL
1	B	46	ILE
1	B	47	GLU
1	B	58	LYS
1	B	79	ASP
1	B	80	GLU
1	B	84	GLU
1	B	87	LYS
1	B	99	ILE
1	B	100	ARG
1	B	119	ARG
1	B	126	LYS
1	B	164	LYS
1	B	165	VAL
1	B	187	LYS

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Mol	Chain	Res	Type
1	B	190	GLU
1	B	203	LYS
1	B	230	ILE
1	B	233	LYS
1	B	251	ILE
1	B	257	GLN
1	B	276	VAL
1	B	292	THR
1	B	293	SER
1	B	304	GLU
1	B	312	VAL
1	B	317	ARG
1	B	329	PRO
1	B	338	ARG
1	B	372	MET
1	B	386	VAL
1	B	389	SER
1	B	400	LYS
1	B	408	LYS
1	B	409	LEU
1	B	413	LYS
1	C	4	LYS
1	C	5	ILE
1	C	12	GLU
1	C	27	LYS
1	C	28	GLU
1	C	38	ASP
1	C	43	ASP
1	C	52	THR
1	C	73	CYS
1	C	79	ASP
1	C	88	LEU
1	C	91	MET
1	C	98	THR
1	C	100	ARG
1	C	103	LEU
1	C	109	ARG
1	C	112	ILE
1	C	119	ARG
1	C	137	ASP
1	C	140	ARG
1	C	142	THR

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Mol	Chain	Res	Type
1	C	151	LYS
1	C	155	THR
1	C	157	THR
1	C	162	THR
1	C	171	ASN
1	C	174	GLU
1	C	182	MET
1	C	198	GLN
1	C	202	SER
1	C	211	THR
1	C	226	ILE
1	C	233	LYS
1	C	234	GLN
1	C	238	GLN
1	C	250	LEU
1	C	257	GLN
1	C	261	SER
1	C	302	THR
1	C	306	GLU
1	C	314	ARG
1	C	338	ARG
1	C	343	ARG
1	C	346	LEU
1	C	372	MET
1	C	400	LYS
1	C	406	LYS
1	C	408	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	328	ASN
1	B	138	GLN
1	B	283	GLN
1	C	238	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

7 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	NAP	B	501	-	45,52,52	1.52	4 (8%)	56,80,80	1.69	9 (16%)
4	BME	A	502	-	3,3,3	0.37	0	1,2,2	0.22	0
3	NAP	C	501	-	45,52,52	1.49	4 (8%)	56,80,80	1.65	8 (14%)
3	NAP	A	501	-	45,52,52	1.47	3 (6%)	56,80,80	1.61	12 (21%)
2	LJY	A	500	-	26,26,26	2.42	4 (15%)	34,36,36	1.58	5 (14%)
2	LJY	B	500	-	26,26,26	2.57	4 (15%)	34,36,36	1.66	5 (14%)
2	LJY	C	500	-	26,26,26	2.39	3 (11%)	34,36,36	1.62	9 (26%)

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	NAP	B	501	-	-	9/31/67/67	0/5/5/5
4	BME	A	502	-	-	1/1/1/1	-
3	NAP	C	501	-	-	10/31/67/67	0/5/5/5
3	NAP	A	501	-	-	10/31/67/67	0/5/5/5
2	LJY	A	500	-	-	0/9/9/9	0/3/3/3
2	LJY	B	500	-	-	1/9/9/9	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LJY	C	500	-	-	1/9/9/9	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	LJY	C3-C18	-11.42	1.27	1.44
2	A	500	LJY	C3-C18	-10.86	1.28	1.44
2	C	500	LJY	C3-C18	-10.82	1.28	1.44
3	B	501	NAP	C4N-C3N	7.67	1.52	1.39
3	C	501	NAP	C4N-C3N	7.42	1.52	1.39
3	A	501	NAP	C4N-C3N	7.29	1.51	1.39
3	C	501	NAP	C5N-C4N	3.94	1.47	1.38
3	A	501	NAP	C5N-C4N	3.86	1.47	1.38
3	B	501	NAP	C5N-C4N	3.60	1.46	1.38
2	B	500	LJY	C6-N1	2.86	1.47	1.38
2	A	500	LJY	C6-N1	2.52	1.46	1.38
2	C	500	LJY	C6-N1	2.38	1.45	1.38
2	A	500	LJY	C15-CL	2.22	1.79	1.74
3	C	501	NAP	C2A-N3A	2.22	1.35	1.32
3	A	501	NAP	C5A-C4A	2.18	1.46	1.40
3	C	501	NAP	C5A-C4A	2.17	1.46	1.40
3	B	501	NAP	C5A-C4A	2.12	1.46	1.40
2	C	500	LJY	C12-N2	2.09	1.36	1.33
2	B	500	LJY	C9-C8	2.06	1.41	1.37
3	B	501	NAP	O4D-C1D	2.05	1.43	1.41
2	A	500	LJY	C9-C8	2.03	1.40	1.37
2	B	500	LJY	C15-CL	2.01	1.78	1.74

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	NAP	C5N-C4N-C3N	-7.23	111.79	120.34
3	B	501	NAP	C5N-C4N-C3N	-6.94	112.14	120.34
3	A	501	NAP	C5N-C4N-C3N	-6.73	112.38	120.34
2	B	500	LJY	C1-O1-C2	5.20	125.39	117.53
2	A	500	LJY	C1-O1-C2	4.60	124.47	117.53
2	C	500	LJY	C1-O1-C2	4.50	124.32	117.53
2	B	500	LJY	C12-N2-C11	4.21	122.62	116.83
3	C	501	NAP	N3A-C2A-N1A	-4.05	122.35	128.68
3	B	501	NAP	N3A-C2A-N1A	-3.67	122.94	128.68
3	B	501	NAP	C3N-C2N-N1N	3.67	124.01	120.43
3	A	501	NAP	C3N-C2N-N1N	3.64	123.99	120.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAP	N3A-C2A-N1A	-3.62	123.02	128.68
2	A	500	LJY	C12-N2-C11	3.36	121.44	116.83
2	A	500	LJY	O1-C2-C3	3.33	119.19	115.50
3	C	501	NAP	C3D-C2D-C1D	3.31	105.96	100.98
3	B	501	NAP	PN-O3-PA	-3.24	121.71	132.83
2	C	500	LJY	C12-N2-C11	3.22	121.25	116.83
3	C	501	NAP	C3N-C2N-N1N	3.07	123.43	120.43
3	A	501	NAP	C3N-C7N-N7N	3.00	121.35	117.75
2	B	500	LJY	C10-C11-N2	-2.89	118.44	122.41
2	A	500	LJY	C8-C12-N2	-2.80	121.14	125.25
3	C	501	NAP	PN-O3-PA	-2.78	123.28	132.83
3	B	501	NAP	C6N-N1N-C2N	-2.75	119.47	121.97
3	A	501	NAP	O7N-C7N-N7N	-2.71	118.72	122.58
2	C	500	LJY	C10-C11-N2	-2.66	118.76	122.41
2	B	500	LJY	C8-C12-N2	-2.55	121.52	125.25
2	C	500	LJY	C8-C12-N2	-2.53	121.54	125.25
3	B	501	NAP	C3D-C2D-C1D	2.53	104.78	100.98
2	C	500	LJY	C16-C15-CL	-2.38	116.66	119.64
3	B	501	NAP	C3N-C7N-N7N	2.37	120.60	117.75
3	C	501	NAP	N6A-C6A-N1A	2.27	123.28	118.57
3	A	501	NAP	O3X-P2B-O1X	2.25	119.48	110.68
3	B	501	NAP	C4A-C5A-N7A	-2.25	107.06	109.40
3	A	501	NAP	C6N-C5N-C4N	2.20	122.63	119.44
3	A	501	NAP	C4A-C5A-N7A	-2.19	107.11	109.40
2	C	500	LJY	C9-C8-C12	2.18	117.89	115.46
2	A	500	LJY	C9-C8-C12	2.11	117.81	115.46
3	A	501	NAP	N6A-C6A-N1A	2.10	122.93	118.57
2	C	500	LJY	C9-C10-C11	2.08	120.99	118.27
2	B	500	LJY	C8-C7-N1	-2.08	108.65	113.03
3	C	501	NAP	C6N-C5N-C4N	2.08	122.45	119.44
3	B	501	NAP	C6N-C5N-C4N	2.07	122.45	119.44
3	A	501	NAP	C2A-N1A-C6A	2.06	122.27	118.75
2	C	500	LJY	O1-C2-C3	2.04	117.76	115.50
3	A	501	NAP	PN-O3-PA	-2.02	125.88	132.83
2	C	500	LJY	C14-C15-CL	2.01	122.50	119.35
3	A	501	NAP	C6N-N1N-C2N	-2.00	120.15	121.97
3	C	501	NAP	O4D-C4D-C3D	2.00	109.07	105.11

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	501	NAP	O4D-C1D-N1N-C2N
3	B	501	NAP	O4D-C1D-N1N-C6N
3	B	501	NAP	C2D-C1D-N1N-C2N
3	B	501	NAP	C2D-C1D-N1N-C6N
4	A	502	BME	O1-C1-C2-S2
3	C	501	NAP	C5D-O5D-PN-O2N
3	C	501	NAP	O4D-C4D-C5D-O5D
3	C	501	NAP	C3D-C4D-C5D-O5D
3	C	501	NAP	O4D-C1D-N1N-C6N
3	A	501	NAP	C5D-O5D-PN-O2N
3	A	501	NAP	O4D-C1D-N1N-C2N
3	A	501	NAP	O4D-C1D-N1N-C6N
3	A	501	NAP	C2D-C1D-N1N-C2N
3	A	501	NAP	C2D-C1D-N1N-C6N
2	C	500	LJY	N3-C18-C3-C2
3	B	501	NAP	O4B-C4B-C5B-O5B
3	B	501	NAP	O4D-C4D-C5D-O5D
3	B	501	NAP	C3D-C4D-C5D-O5D
3	B	501	NAP	C3B-C4B-C5B-O5B
3	C	501	NAP	C2N-C3N-C7N-N7N
3	C	501	NAP	C2N-C3N-C7N-O7N
3	A	501	NAP	O4B-C4B-C5B-O5B
3	C	501	NAP	C4N-C3N-C7N-N7N
3	A	501	NAP	PN-O3-PA-O5B
3	B	501	NAP	C5B-O5B-PA-O3
3	C	501	NAP	C5D-O5D-PN-O3
3	A	501	NAP	C5D-O5D-PN-O3
3	C	501	NAP	C4N-C3N-C7N-O7N
3	C	501	NAP	C5D-O5D-PN-O1N
3	A	501	NAP	C5D-O5D-PN-O1N
3	A	501	NAP	C3B-C4B-C5B-O5B
2	B	500	LJY	N3-C18-C3-C2

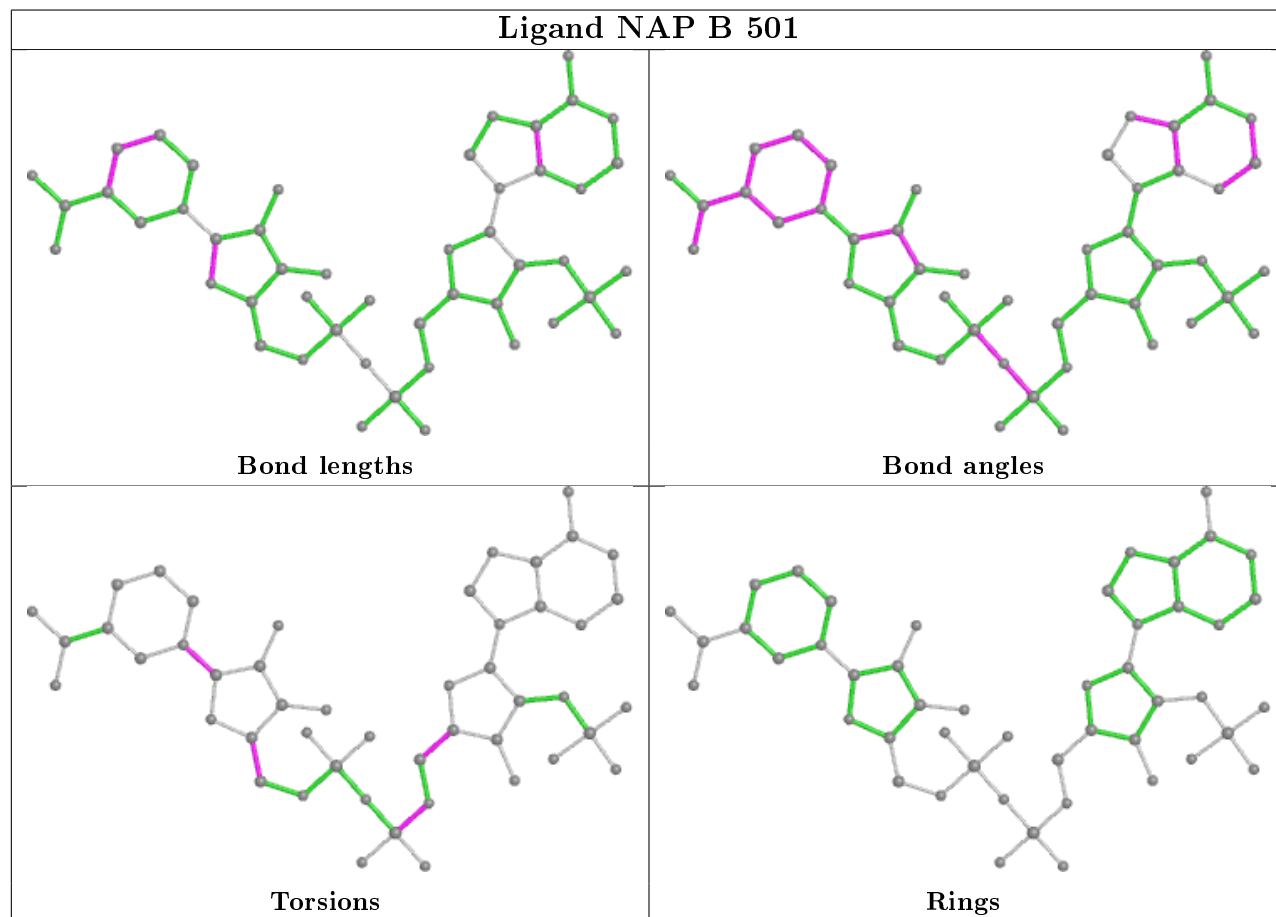
There are no ring outliers.

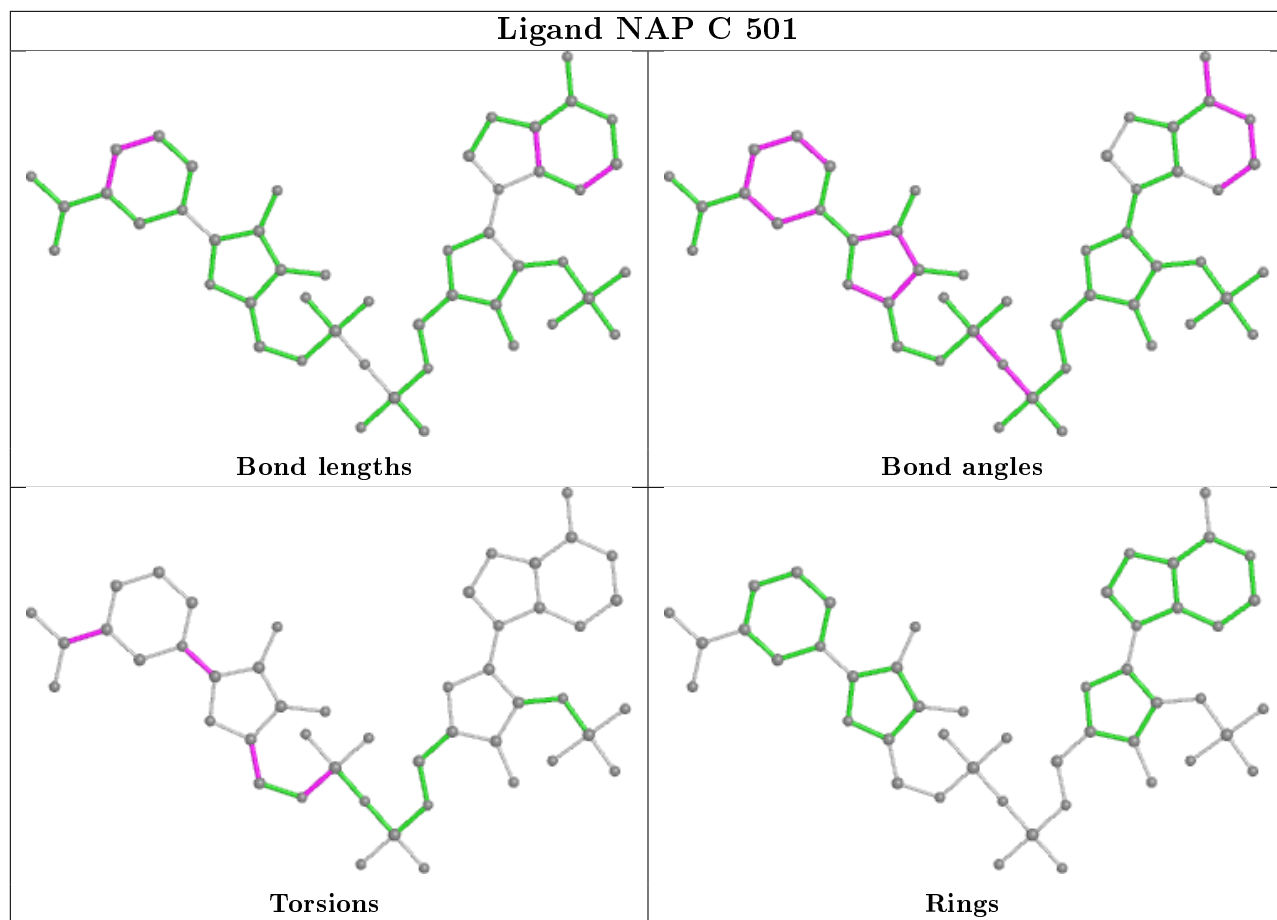
3 monomers are involved in 3 short contacts:

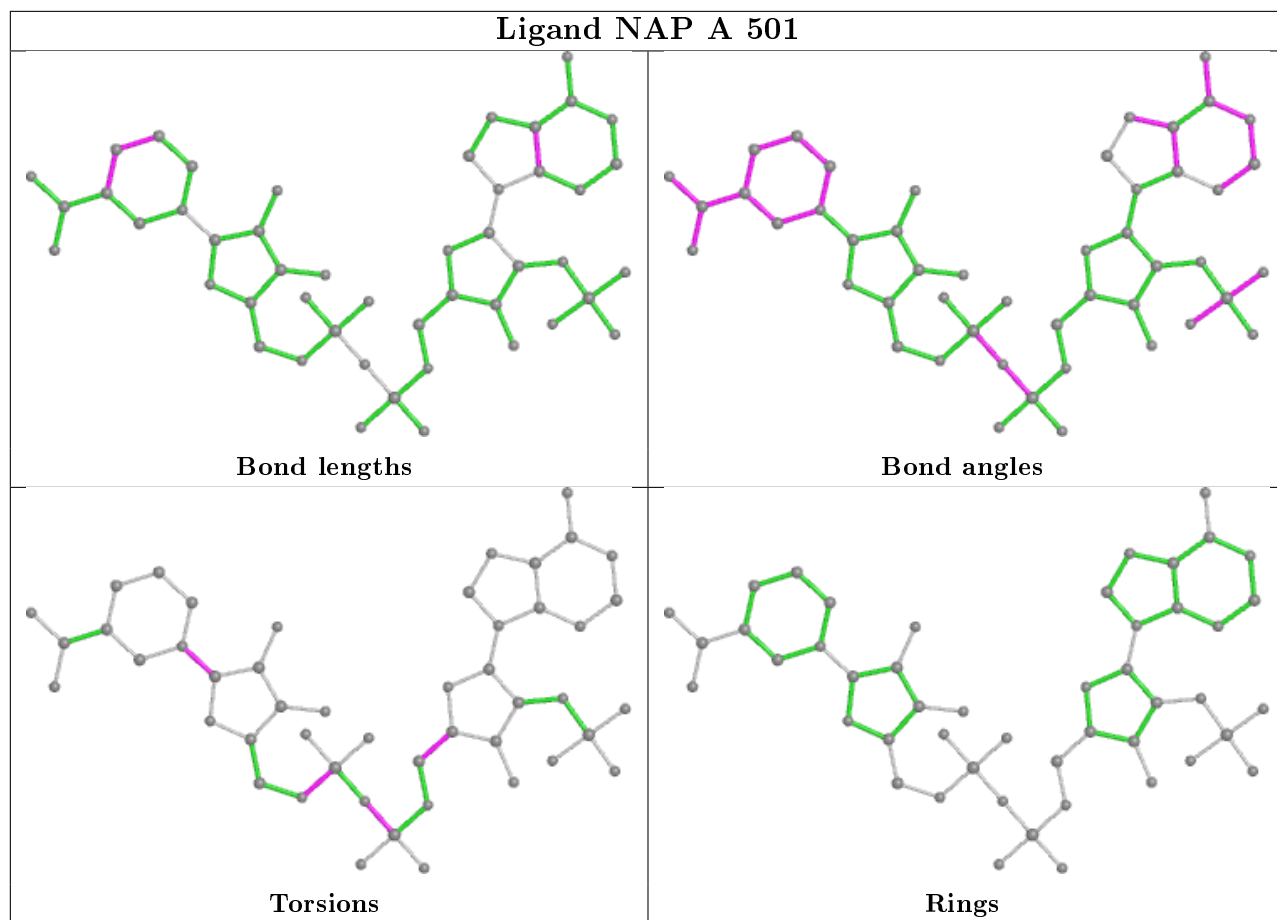
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	BME	1	0
3	A	501	NAP	1	0
2	B	500	LJY	1	0

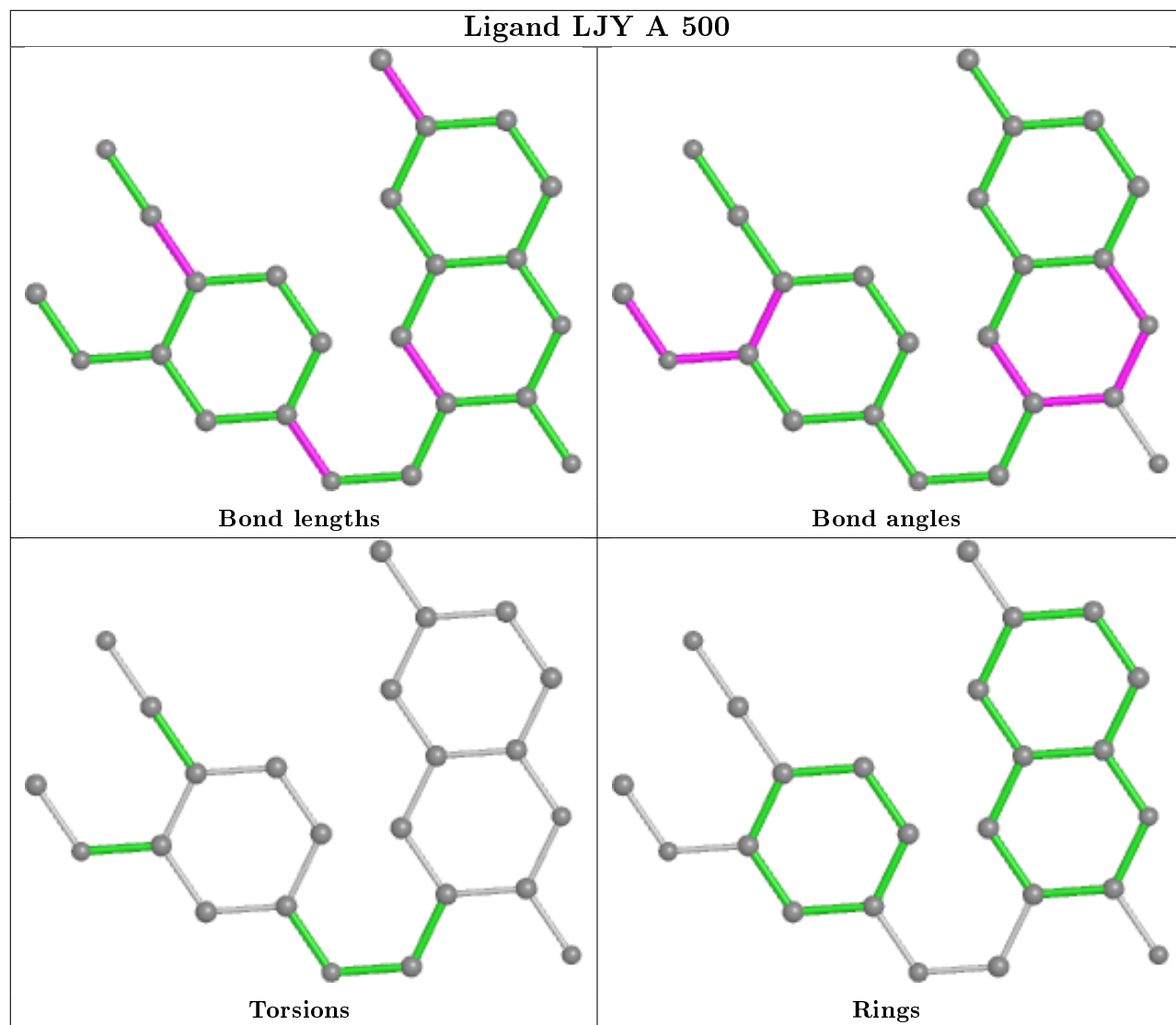
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

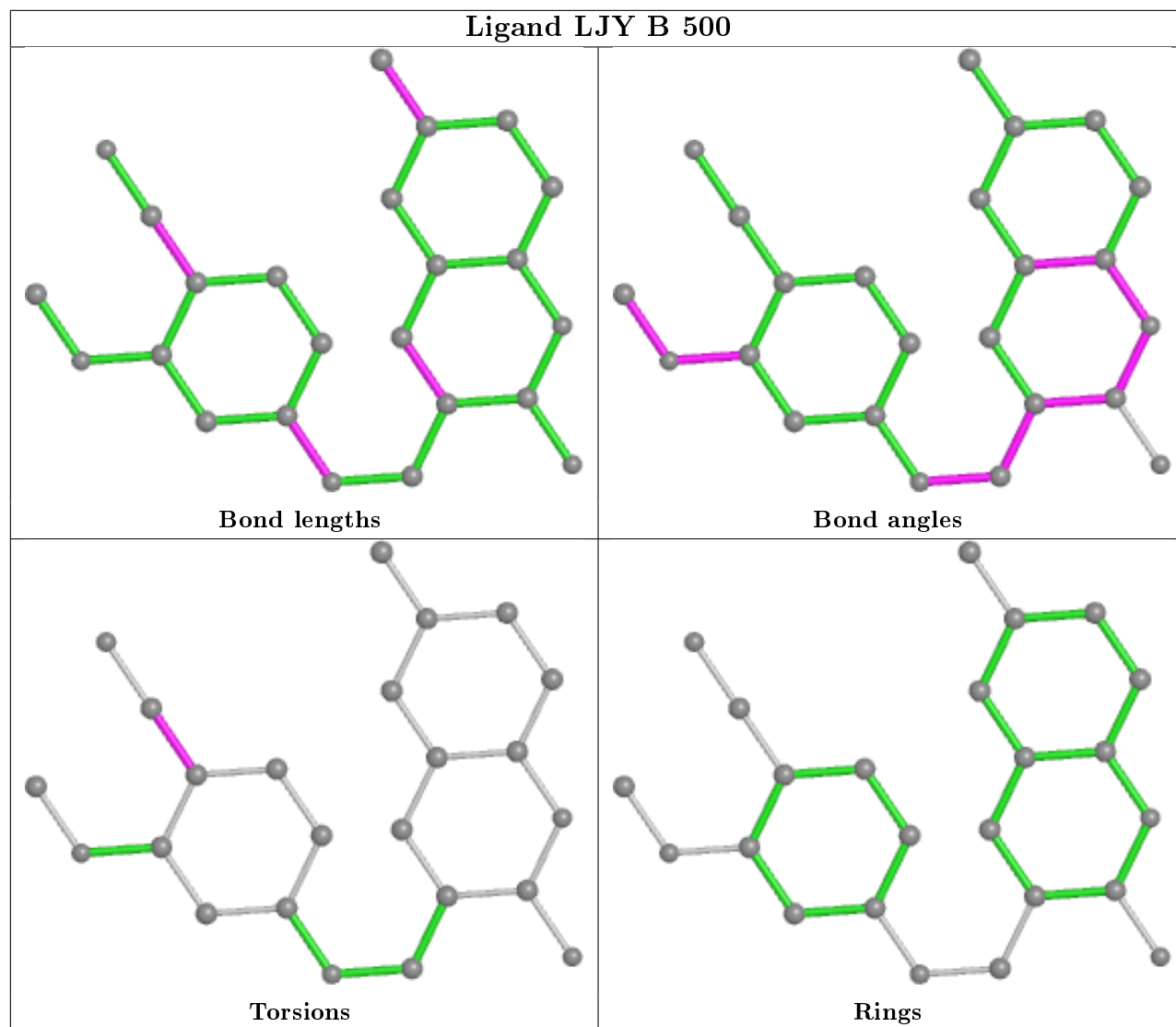
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

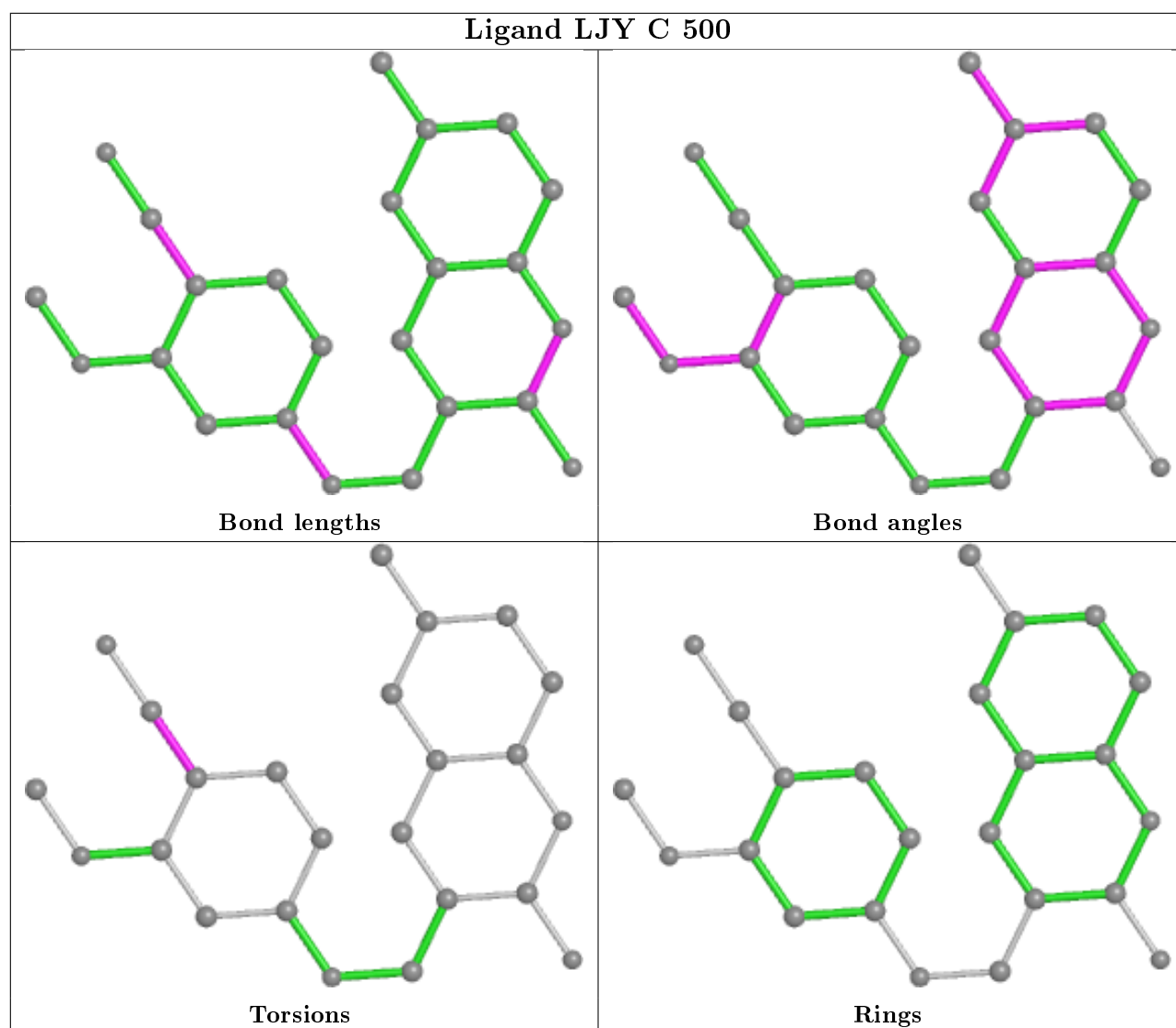












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	413/425 (97%)	-0.37	0 100 100	49, 71, 95, 120	0
1	B	411/425 (96%)	-0.27	0 100 100	53, 78, 105, 125	0
1	C	409/425 (96%)	0.07	21 (5%) 28 19	67, 101, 153, 179	0
All	All	1233/1275 (96%)	-0.19	21 (1%) 70 63	49, 81, 123, 179	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	ILE	3.8
1	C	54	ASP	3.5
1	C	164	LYS	3.3
1	C	145	VAL	3.2
1	C	166	THR	2.9
1	C	146	VAL	2.9
1	C	163	GLN	2.8
1	C	165	VAL	2.8
1	C	170	HIS	2.8
1	C	148	GLY	2.8
1	C	90	GLN	2.7
1	C	168	LEU	2.6
1	C	151	LYS	2.5
1	C	410	ALA	2.4
1	C	160	ASP	2.3
1	C	144	PHE	2.3
1	C	156	TYR	2.3
1	C	355	PHE	2.2
1	C	51	ALA	2.2
1	C	87	LYS	2.1
1	C	414	LEU	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

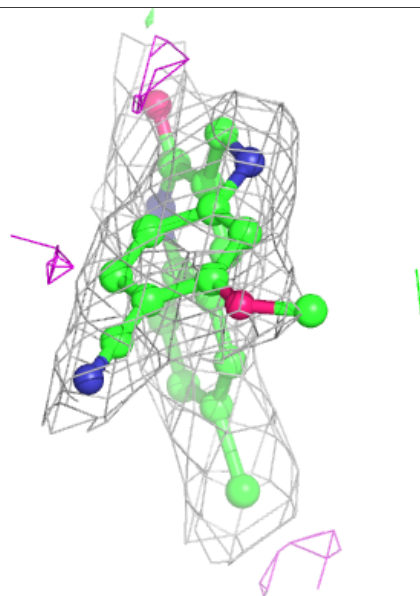
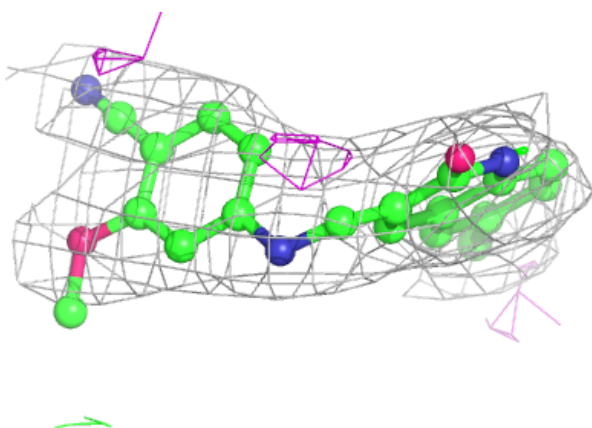
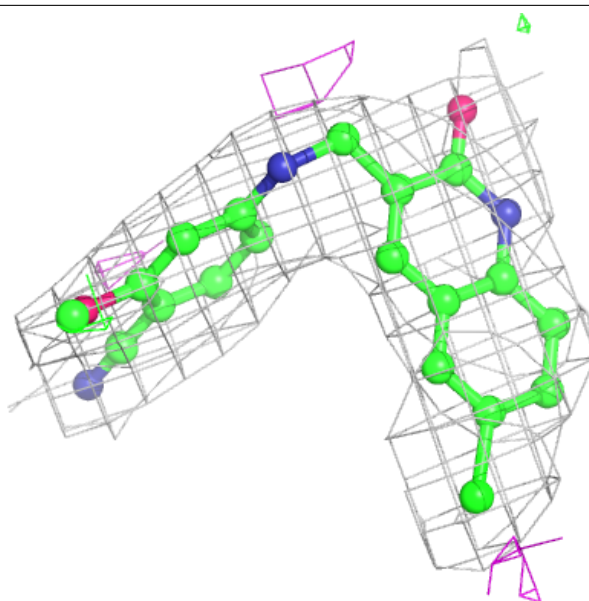
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BME	A	502	4/4	0.88	0.31	67,69,71,78	0
2	LJY	C	500	24/24	0.93	0.19	55,66,72,76	0
2	LJY	A	500	24/24	0.95	0.19	69,73,79,81	0
3	NAP	C	501	48/48	0.95	0.17	51,79,93,97	0
2	LJY	B	500	24/24	0.96	0.18	47,48,55,59	0
3	NAP	B	501	48/48	0.96	0.14	54,68,76,82	0
3	NAP	A	501	48/48	0.97	0.14	51,56,67,75	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.

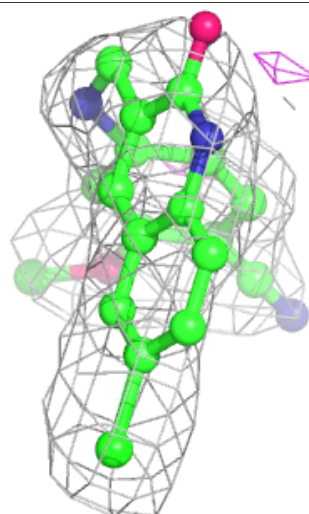
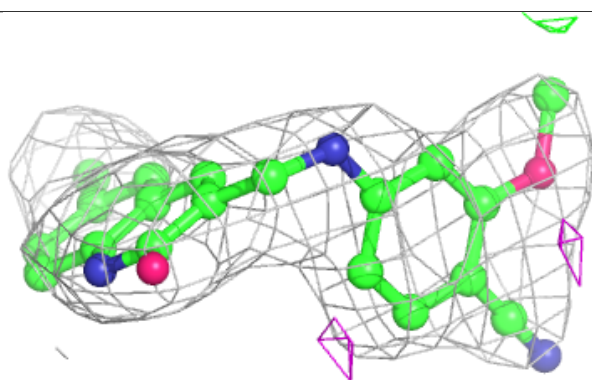
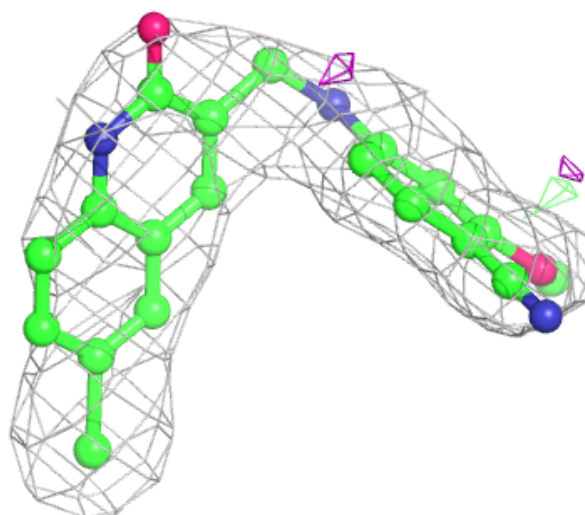
Electron density around LJY C 500:

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



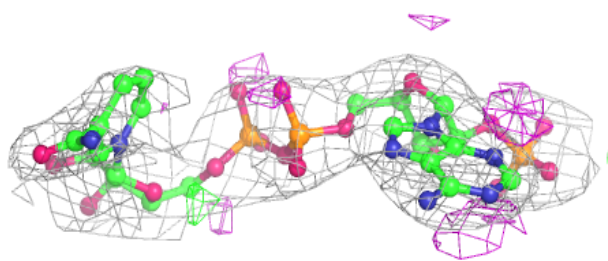
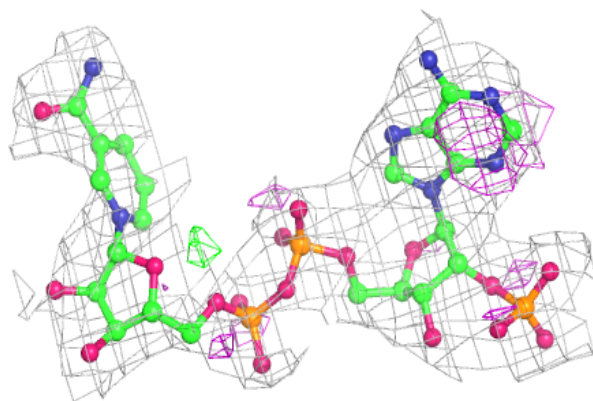
Electron density around LJY A 500:

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



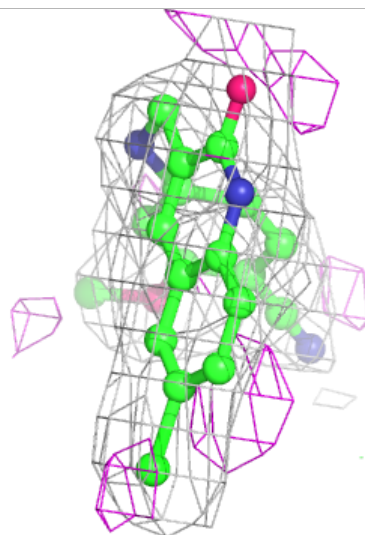
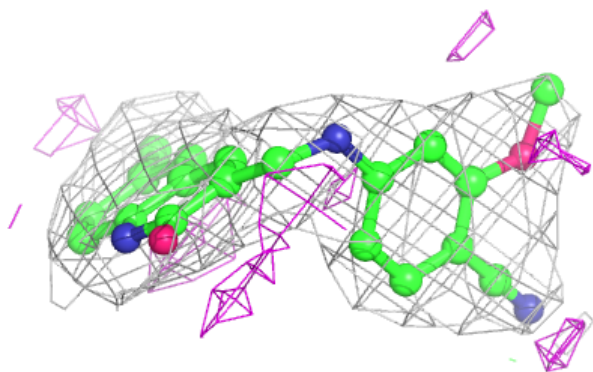
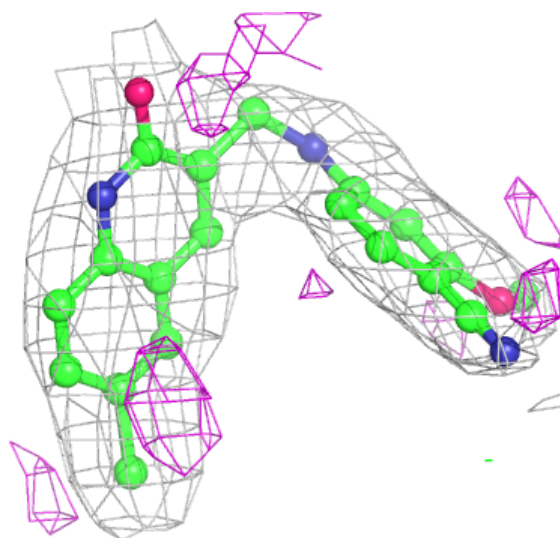
Electron density around NAP C 501:

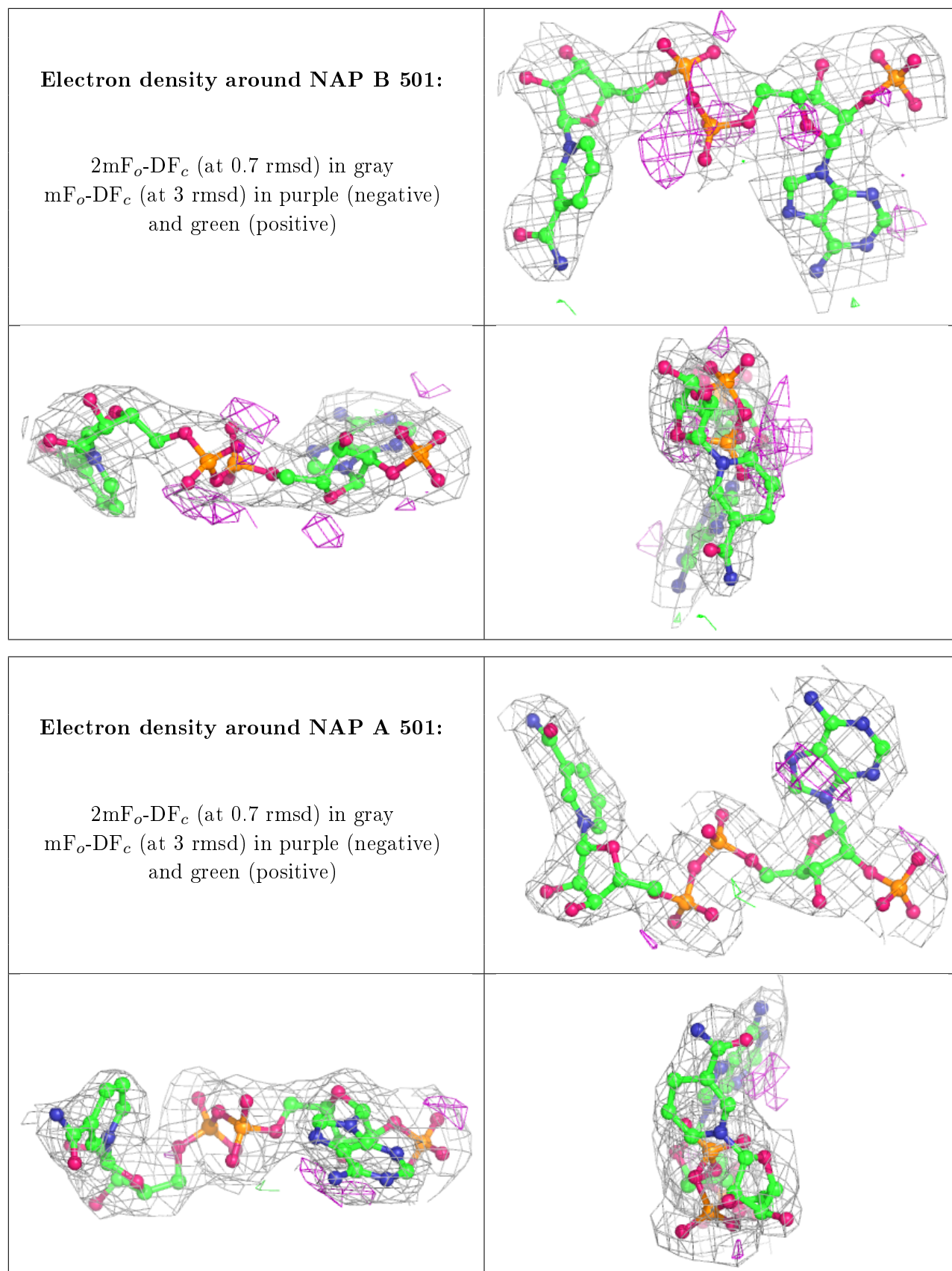
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around LJY B 500:

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





6.5 Other polymers

There are no such residues in this entry.