



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:20 AM UTC

PDB ID : 7CMP / pdb_00007cmp
Title : parE in complex with AMPPNP
Authors : Jung, H.Y.; Heo, Y.-S.
Deposited on : 2020-07-28
Resolution : 2.89 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

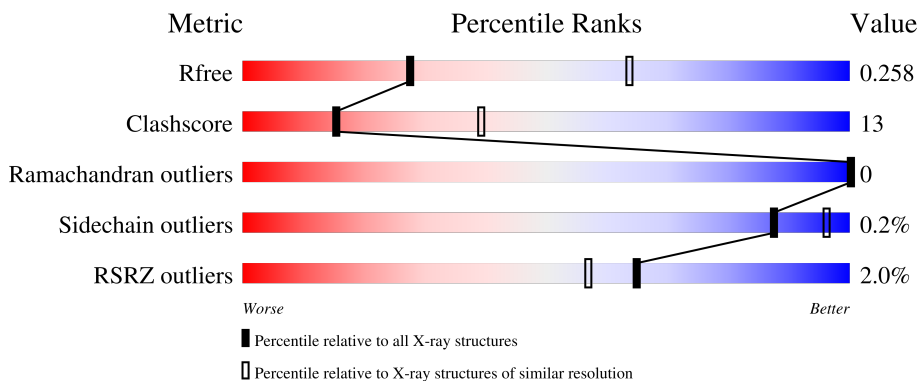
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



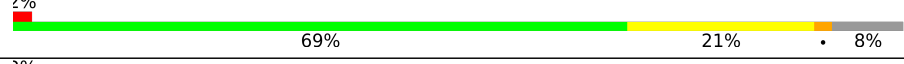

The reported resolution of this entry is 2.89 Å.

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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	408	 2% 69% 21% • 8%
1	B	408	 2% 67% 23% • 8%
1	C	408	 2% 69% 21% • 8%
1	D	408	 2% 69% 21% • 8%

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 11878 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 DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	374	2923	1837	522	555	9	0	0	0
1	B	374	2923	1837	522	555	9	0	0	0
1	C	374	2923	1837	522	555	9	0	0	0
1	D	374	2923	1837	522	555	9	0	0	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP Q5GYJ8
A	27	GLY	-	expression tag	UNP Q5GYJ8
A	28	SER	-	expression tag	UNP Q5GYJ8
A	29	SER	-	expression tag	UNP Q5GYJ8
A	30	HIS	-	expression tag	UNP Q5GYJ8
A	31	HIS	-	expression tag	UNP Q5GYJ8
A	32	HIS	-	expression tag	UNP Q5GYJ8
A	33	HIS	-	expression tag	UNP Q5GYJ8
A	34	HIS	-	expression tag	UNP Q5GYJ8
A	35	HIS	-	expression tag	UNP Q5GYJ8
A	36	SER	-	expression tag	UNP Q5GYJ8
A	37	SER	-	expression tag	UNP Q5GYJ8
A	38	GLY	-	expression tag	UNP Q5GYJ8
A	39	LEU	-	expression tag	UNP Q5GYJ8
A	40	VAL	-	expression tag	UNP Q5GYJ8
A	41	PRO	-	expression tag	UNP Q5GYJ8
A	42	ARG	-	expression tag	UNP Q5GYJ8
A	43	GLY	-	expression tag	UNP Q5GYJ8
A	44	SER	-	expression tag	UNP Q5GYJ8
A	45	HIS	-	expression tag	UNP Q5GYJ8
B	26	MET	-	initiating methionine	UNP Q5GYJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	GLY	-	expression tag	UNP Q5GYJ8
B	28	SER	-	expression tag	UNP Q5GYJ8
B	29	SER	-	expression tag	UNP Q5GYJ8
B	30	HIS	-	expression tag	UNP Q5GYJ8
B	31	HIS	-	expression tag	UNP Q5GYJ8
B	32	HIS	-	expression tag	UNP Q5GYJ8
B	33	HIS	-	expression tag	UNP Q5GYJ8
B	34	HIS	-	expression tag	UNP Q5GYJ8
B	35	HIS	-	expression tag	UNP Q5GYJ8
B	36	SER	-	expression tag	UNP Q5GYJ8
B	37	SER	-	expression tag	UNP Q5GYJ8
B	38	GLY	-	expression tag	UNP Q5GYJ8
B	39	LEU	-	expression tag	UNP Q5GYJ8
B	40	VAL	-	expression tag	UNP Q5GYJ8
B	41	PRO	-	expression tag	UNP Q5GYJ8
B	42	ARG	-	expression tag	UNP Q5GYJ8
B	43	GLY	-	expression tag	UNP Q5GYJ8
B	44	SER	-	expression tag	UNP Q5GYJ8
B	45	HIS	-	expression tag	UNP Q5GYJ8
C	26	MET	-	initiating methionine	UNP Q5GYJ8
C	27	GLY	-	expression tag	UNP Q5GYJ8
C	28	SER	-	expression tag	UNP Q5GYJ8
C	29	SER	-	expression tag	UNP Q5GYJ8
C	30	HIS	-	expression tag	UNP Q5GYJ8
C	31	HIS	-	expression tag	UNP Q5GYJ8
C	32	HIS	-	expression tag	UNP Q5GYJ8
C	33	HIS	-	expression tag	UNP Q5GYJ8
C	34	HIS	-	expression tag	UNP Q5GYJ8
C	35	HIS	-	expression tag	UNP Q5GYJ8
C	36	SER	-	expression tag	UNP Q5GYJ8
C	37	SER	-	expression tag	UNP Q5GYJ8
C	38	GLY	-	expression tag	UNP Q5GYJ8
C	39	LEU	-	expression tag	UNP Q5GYJ8
C	40	VAL	-	expression tag	UNP Q5GYJ8
C	41	PRO	-	expression tag	UNP Q5GYJ8
C	42	ARG	-	expression tag	UNP Q5GYJ8
C	43	GLY	-	expression tag	UNP Q5GYJ8
C	44	SER	-	expression tag	UNP Q5GYJ8
C	45	HIS	-	expression tag	UNP Q5GYJ8
D	26	MET	-	initiating methionine	UNP Q5GYJ8
D	27	GLY	-	expression tag	UNP Q5GYJ8
D	28	SER	-	expression tag	UNP Q5GYJ8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	29	SER	-	expression tag	UNP Q5GYJ8
D	30	HIS	-	expression tag	UNP Q5GYJ8
D	31	HIS	-	expression tag	UNP Q5GYJ8
D	32	HIS	-	expression tag	UNP Q5GYJ8
D	33	HIS	-	expression tag	UNP Q5GYJ8
D	34	HIS	-	expression tag	UNP Q5GYJ8
D	35	HIS	-	expression tag	UNP Q5GYJ8
D	36	SER	-	expression tag	UNP Q5GYJ8
D	37	SER	-	expression tag	UNP Q5GYJ8
D	38	GLY	-	expression tag	UNP Q5GYJ8
D	39	LEU	-	expression tag	UNP Q5GYJ8
D	40	VAL	-	expression tag	UNP Q5GYJ8
D	41	PRO	-	expression tag	UNP Q5GYJ8
D	42	ARG	-	expression tag	UNP Q5GYJ8
D	43	GLY	-	expression tag	UNP Q5GYJ8
D	44	SER	-	expression tag	UNP Q5GYJ8
D	45	HIS	-	expression tag	UNP Q5GYJ8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

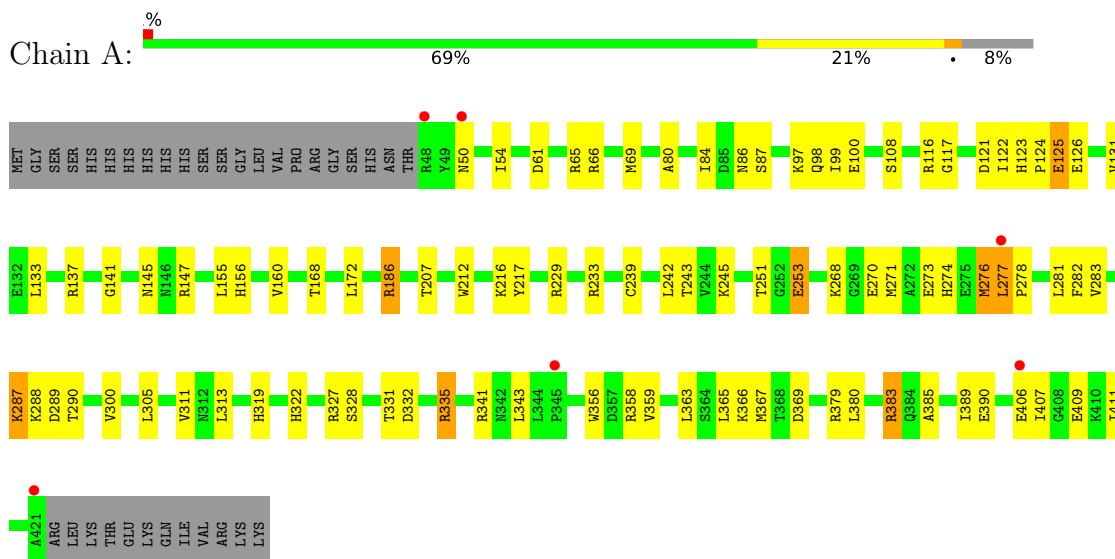
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃) (labeled as "Ligand of Interest" by depositor).

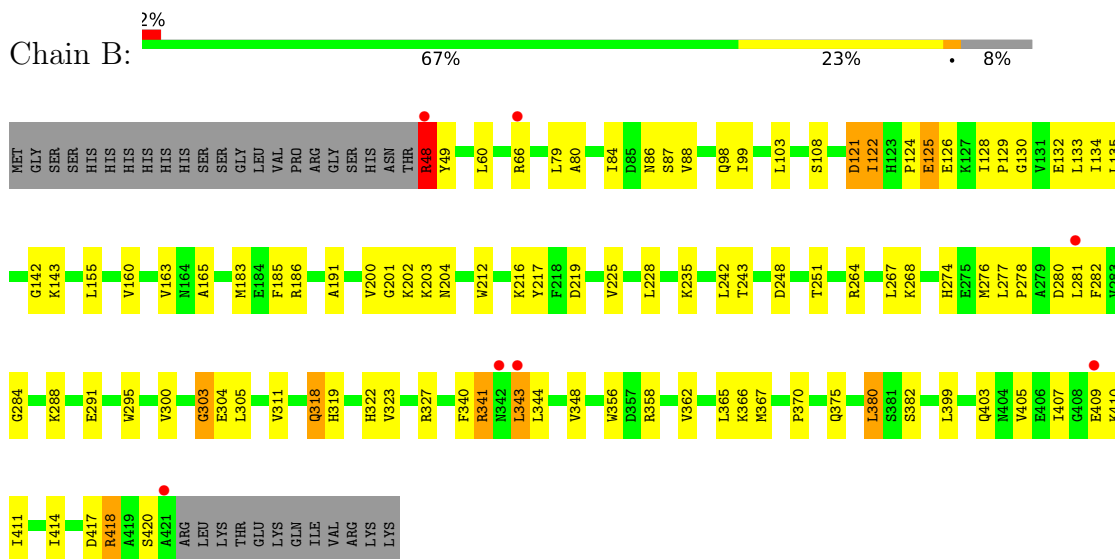
3 Residue-property plots

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

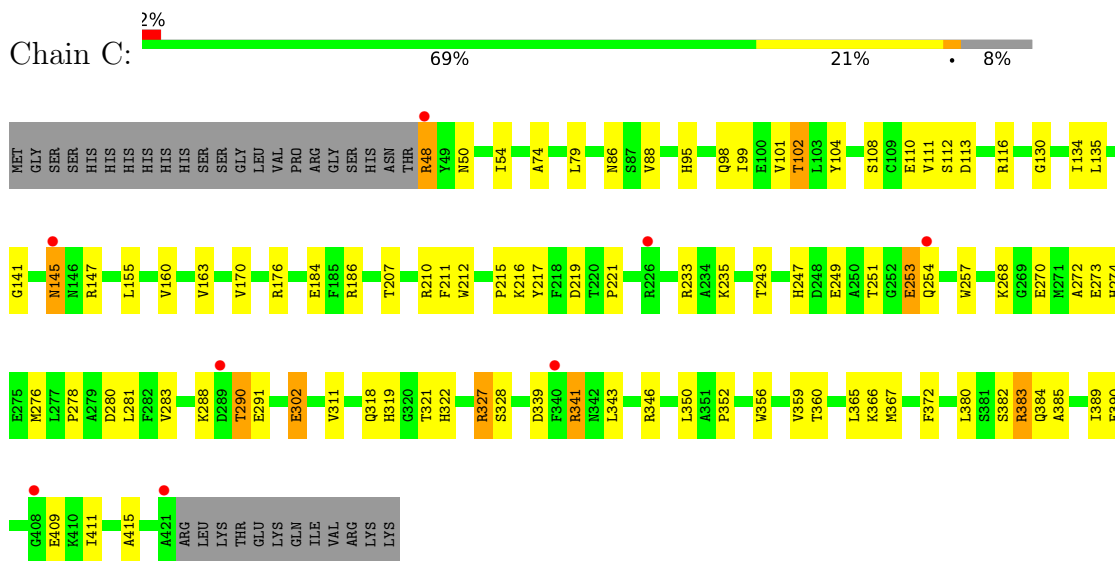
- Molecule 1: DNA topoisomerase 4 subunit B



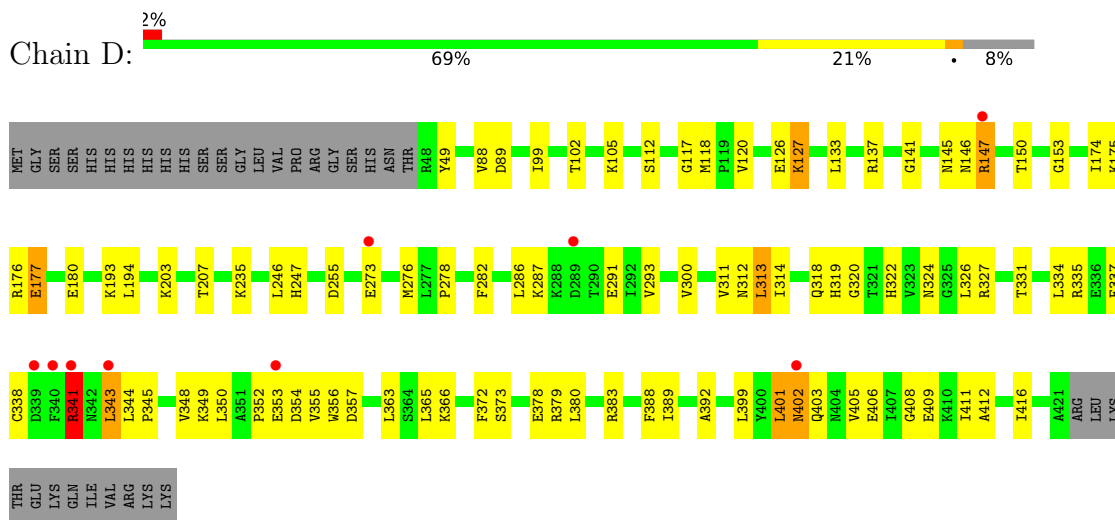
- Molecule 1: DNA topoisomerase 4 subunit B



- Molecule 1: DNA topoisomerase 4 subunit B



• Molecule 1: DNA topoisomerase 4 subunit B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.02Å 126.75Å 96.04Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	46.10 – 2.89 46.10 – 2.89	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.10-2.89) 98.5 (46.10-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.91Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.202 , 0.260 0.202 , 0.258	Depositor DCC
R_{free} test set	1847 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	47.3	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.3	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	0.92	EDS
Total number of atoms	11878	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: MG, ANP

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	0.41	1/2983 (0.0%)	0.89	18/4036 (0.4%)
1	B	0.49	4/2983 (0.1%)	0.86	20/4036 (0.5%)
1	C	0.39	1/2983 (0.0%)	0.84	17/4036 (0.4%)
1	D	0.49	2/2983 (0.1%)	0.90	26/4036 (0.6%)
All	All	0.45	8/11932 (0.1%)	0.87	81/16144 (0.5%)

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	B	0	3
1	C	0	1
1	D	0	1
All	All	0	5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	48	ARG	CD-NE	-7.30	1.36	1.46
1	B	288	LYS	CD-CE	7.09	1.73	1.52
1	B	122	ILE	CG1-CD1	6.17	1.75	1.51
1	B	121	ASP	C-N	5.93	1.40	1.33
1	D	273	GLU	CD-OE2	5.89	1.36	1.25
1	D	203	LYS	CG-CD	5.59	1.69	1.52
1	C	383	ARG	CG-CD	-5.58	1.35	1.52
1	A	253	GLU	CD-OE2	5.32	1.35	1.25

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	186	ARG	CB-CG-CD	-13.05	81.29	111.30
1	D	273	GLU	CA-CB-CG	-12.04	90.02	114.10
1	A	186	ARG	CG-CD-NE	11.54	137.40	112.00
1	A	186	ARG	NE-CZ-NH2	-11.43	108.92	119.20
1	A	287	LYS	CB-CG-CD	-11.36	85.17	111.30
1	C	383	ARG	CB-CG-CD	-11.09	85.80	111.30
1	C	253	GLU	CA-CB-CG	-10.92	92.26	114.10
1	A	186	ARG	CD-NE-CZ	10.07	138.50	124.40
1	D	343	LEU	CB-CG-CD2	-9.72	81.53	110.70
1	B	48	ARG	NE-CZ-NH2	-9.72	110.45	119.20
1	C	145	ASN	CB-CA-C	-9.55	97.99	113.37
1	B	409	GLU	CA-CB-CG	-9.47	95.16	114.10
1	B	288	LYS	CG-CD-CE	-9.36	89.76	111.30
1	D	105	LYS	CB-CA-C	-9.11	93.77	110.63
1	B	343	LEU	CA-CB-CG	-8.80	85.52	116.30
1	A	287	LYS	CA-CB-CG	8.76	131.61	114.10
1	D	341	ARG	CA-CB-CG	-8.70	96.71	114.10
1	A	97	LYS	CD-CE-NZ	8.62	139.47	111.90
1	D	147	ARG	CA-CB-CG	8.45	130.99	114.10
1	B	125	GLU	CA-CB-CG	-8.19	97.72	114.10
1	A	287	LYS	CG-CD-CE	7.89	129.44	111.30
1	D	287	LYS	CB-CG-CD	-7.88	93.18	111.30
1	C	384	GLN	CB-CG-CD	-7.86	99.25	112.60
1	B	125	GLU	CG-CD-OE1	-7.75	100.58	118.40
1	D	127	LYS	N-CA-CB	-7.66	105.44	114.17
1	B	203	LYS	CG-CD-CE	-7.64	93.72	111.30
1	D	177	GLU	CA-CB-CG	-7.13	99.84	114.10
1	D	273	GLU	CB-CA-C	-7.11	95.14	109.99
1	C	383	ARG	N-CA-C	-7.09	104.10	112.89
1	A	50	ASN	CB-CA-C	-7.03	97.02	111.22
1	B	48	ARG	CG-CD-NE	6.98	127.36	112.00
1	B	304	GLU	CA-CB-CG	-6.98	100.14	114.10
1	C	341	ARG	CG-CD-NE	-6.95	96.71	112.00
1	B	418	ARG	N-CA-CB	-6.95	99.60	110.30
1	D	273	GLU	CB-CG-CD	6.83	124.21	112.60
1	D	147	ARG	CG-CD-NE	-6.82	97.00	112.00
1	C	290	THR	CA-C-N	6.80	133.21	121.64
1	C	290	THR	C-N-CA	6.80	133.21	121.64
1	D	341	ARG	CG-CD-NE	-6.72	97.21	112.00
1	B	341	ARG	CB-CG-CD	-6.67	95.95	111.30
1	B	48	ARG	CA-CB-CG	-6.54	101.02	114.10
1	C	48	ARG	N-CA-C	-6.35	93.21	111.00
1	B	48	ARG	CD-NE-CZ	6.30	133.21	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	ARG	CA-CB-CG	6.29	126.67	114.10
1	D	401	LEU	CA-C-N	6.26	129.82	120.31
1	D	401	LEU	C-N-CA	6.26	129.82	120.31
1	D	105	LYS	N-CA-CB	6.16	119.71	110.22
1	A	287	LYS	N-CA-CB	6.03	120.40	110.69
1	D	273	GLU	CG-CD-OE1	-5.92	104.77	118.40
1	A	383	ARG	NE-CZ-NH1	-5.91	115.59	121.50
1	D	147	ARG	CD-NE-CZ	5.88	132.63	124.40
1	A	125	GLU	CA-CB-CG	-5.86	102.38	114.10
1	B	122	ILE	CG1-CB-CG2	-5.85	93.15	110.70
1	A	277	LEU	CB-CG-CD2	5.82	128.17	110.70
1	D	341	ARG	CB-CG-CD	5.79	124.61	111.30
1	A	335	ARG	CB-CG-CD	-5.77	98.03	111.30
1	D	402	ASN	N-CA-CB	-5.54	101.69	110.28
1	B	48	ARG	N-CA-C	5.54	126.52	111.00
1	D	203	LYS	CA-CB-CG	5.48	125.07	114.10
1	D	406	GLU	CB-CA-C	5.39	121.02	110.67
1	C	383	ARG	CG-CD-NE	5.36	123.78	112.00
1	B	203	LYS	CD-CE-NZ	5.34	129.00	111.90
1	D	409	GLU	N-CA-CB	-5.33	100.66	109.72
1	A	406	GLU	CA-CB-CG	-5.33	103.45	114.10
1	D	287	LYS	N-CA-CB	-5.32	102.35	110.65
1	C	272	ALA	CA-C-N	-5.32	113.77	122.54
1	C	272	ALA	C-N-CA	-5.32	113.77	122.54
1	B	303	GLY	CA-C-N	-5.27	115.28	122.93
1	B	303	GLY	C-N-CA	-5.27	115.28	122.93
1	C	341	ARG	N-CA-CB	-5.27	103.46	111.15
1	A	287	LYS	CB-CA-C	-5.26	99.92	109.38
1	C	254	GLN	CB-CA-C	5.24	119.72	109.35
1	D	313	LEU	CA-C-N	-5.23	118.22	123.04
1	D	313	LEU	C-N-CA	-5.23	118.22	123.04
1	A	186	ARG	NE-CZ-NH1	5.23	126.73	121.50
1	C	341	ARG	NE-CZ-NH1	-5.23	116.27	121.50
1	C	273	GLU	N-CA-CB	5.23	118.23	110.49
1	C	327	ARG	NE-CZ-NH1	-5.22	116.28	121.50
1	A	276	MET	CB-CG-SD	-5.14	97.27	112.70
1	B	341	ARG	CG-CD-NE	5.14	123.31	112.00
1	D	287	LYS	CB-CA-C	5.03	118.50	110.16

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	318	GLN	Peptide
1	B	48	ARG	Peptide,Sidechain
1	C	302	GLU	Peptide
1	D	341	ARG	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2923	0	2875	78	0
1	B	2923	0	2874	86	0
1	C	2923	0	2875	72	0
1	D	2923	0	2874	98	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	31	0	12	2	0
3	B	31	0	13	2	0
3	C	31	0	12	3	0
3	D	31	0	12	2	0
4	A	28	0	0	5	0
4	B	7	0	0	0	0
4	C	16	0	0	0	0
4	D	7	0	0	0	0
All	All	11878	0	11547	315	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 13.

All (315) 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:B:122:ILE:CD1	1:B:122:ILE:CG1	1.75	1.54
1:A:155:LEU:HD12	1:B:66:ARG:NE	1.51	1.22
1:D:176:ARG:HB2	1:D:177:GLU:OE1	1.43	1.16
1:A:379:ARG:NH2	1:B:318:GLN:OE1	1.83	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LEU:HD12	1:B:66:ARG:HE	1.13	1.01
1:C:276:MET:HE3	1:C:360:THR:HG21	1.43	0.99
1:A:383:ARG:CD	4:A:602:HOH:O	2.12	0.98
1:A:66:ARG:HE	1:B:155:LEU:HB2	1.30	0.96
1:A:271:MET:HB2	1:A:276:MET:HE3	1.48	0.95
1:D:176:ARG:CB	1:D:177:GLU:OE1	2.18	0.91
1:A:383:ARG:HD3	4:A:602:HOH:O	1.68	0.91
1:B:341:ARG:NH2	1:B:405:VAL:HG21	1.85	0.91
1:B:186:ARG:HD2	1:B:191:ALA:CB	2.04	0.88
1:B:276:MET:HE1	1:B:281:LEU:HG	1.54	0.87
1:C:383:ARG:HD2	1:C:383:ARG:C	2.00	0.86
1:D:337:PHE:O	1:D:341:ARG:HB2	1.76	0.86
1:D:353:GLU:HG2	1:D:354:ASP:N	1.92	0.85
1:A:379:ARG:HH22	1:B:318:GLN:CD	1.84	0.84
1:B:186:ARG:HD2	1:B:191:ALA:HB1	1.60	0.82
1:B:264:ARG:NH1	1:B:280:ASP:O	2.12	0.82
1:A:327:ARG:HD3	1:A:356:TRP:CG	2.13	0.82
1:C:276:MET:CE	1:C:360:THR:HG21	2.08	0.82
1:D:276:MET:HG2	1:D:300:VAL:HG22	1.61	0.81
1:C:341:ARG:HB3	1:C:343:LEU:HD13	1.62	0.81
1:A:87:SER:HB3	1:A:99:ILE:HD12	1.63	0.80
1:C:268:LYS:NZ	1:C:280:ASP:OD2	2.13	0.80
1:A:332:ASP:OD1	1:A:335:ARG:NH2	2.15	0.80
1:A:168:THR:O	1:A:186:ARG:HD2	1.82	0.79
1:B:87:SER:HB3	1:B:99:ILE:HD12	1.65	0.78
1:A:366:LYS:NZ	4:A:601:HOH:O	2.16	0.78
1:C:184:GLU:OE1	1:C:186:ARG:NH1	2.16	0.78
1:D:193:LYS:HG2	1:D:194:LEU:H	1.48	0.77
1:D:176:ARG:HD3	1:D:177:GLU:OE2	1.85	0.76
1:A:69:MET:HE1	1:B:375:GLN:HG2	1.68	0.75
1:D:343:LEU:HD21	1:D:416:ILE:CD1	2.15	0.75
1:C:327:ARG:HG3	1:C:356:TRP:CD2	2.22	0.75
1:B:341:ARG:HB2	1:B:343:LEU:CD1	2.17	0.75
1:B:341:ARG:HB2	1:B:343:LEU:HD12	1.68	0.75
1:D:399:LEU:O	1:D:403:GLN:HG2	1.88	0.74
1:C:346:ARG:HG2	1:C:346:ARG:HH11	1.53	0.73
1:D:335:ARG:NH1	1:D:350:LEU:O	2.21	0.73
1:D:327:ARG:HD3	1:D:352:PRO:HB3	1.71	0.72
1:B:88:VAL:HG21	1:B:235:LYS:HD2	1.71	0.72
1:D:88:VAL:HG21	1:D:235:LYS:HD2	1.71	0.72
1:A:383:ARG:HD2	4:A:602:HOH:O	1.83	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:HIS:CD2	1:B:303:GLY:HA3	2.25	0.71
1:D:176:ARG:HD3	1:D:177:GLU:CD	2.15	0.71
1:D:353:GLU:HG2	1:D:354:ASP:H	1.56	0.71
1:D:326:LEU:HD12	1:D:363:LEU:HD13	1.74	0.70
1:A:277:LEU:CD2	1:A:411:ILE:HG12	2.22	0.70
1:D:326:LEU:HD22	1:D:356:TRP:HH2	1.57	0.70
1:D:327:ARG:O	1:D:331:THR:HG23	1.92	0.70
1:A:80:ALA:O	1:A:84:ILE:HG12	1.92	0.70
1:A:121:ASP:OD2	1:A:122:ILE:N	2.26	0.69
1:D:193:LYS:HZ2	1:D:194:LEU:HB3	1.57	0.69
1:B:86:ASN:ND2	1:B:160:VAL:HG23	2.08	0.68
1:D:343:LEU:HD21	1:D:416:ILE:HD11	1.75	0.68
1:C:290:THR:O	1:C:291:GLU:HG3	1.94	0.68
1:D:120:VAL:HG22	1:D:176:ARG:HD2	1.78	0.66
1:D:126:GLU:CD	1:D:137:ARG:HH22	2.04	0.66
1:C:319:HIS:O	1:C:322:HIS:NE2	2.29	0.65
1:D:312:ASN:OD1	1:D:366:LYS:HA	1.96	0.65
1:C:339:ASP:C	1:C:341:ARG:H	2.03	0.65
1:C:50:ASN:OD1	1:D:176:ARG:NH1	2.30	0.65
1:A:383:ARG:HD2	1:B:219:ASP:OD1	1.96	0.65
1:A:98:GLN:HG2	1:A:243:THR:HB	1.77	0.64
1:B:380:LEU:HD22	1:B:382:SER:H	1.60	0.64
1:B:80:ALA:O	1:B:84:ILE:HG12	1.97	0.64
1:D:338:CYS:HB3	1:D:344:LEU:HB2	1.78	0.64
1:A:277:LEU:HD22	1:A:411:ILE:HG12	1.79	0.64
1:B:186:ARG:HD2	1:B:191:ALA:HB2	1.78	0.62
1:D:343:LEU:HD23	1:D:343:LEU:C	2.24	0.62
1:C:365:LEU:HD21	1:C:367:MET:HE2	1.81	0.62
1:A:66:ARG:NE	1:B:155:LEU:HB2	2.08	0.61
1:A:86:ASN:ND2	1:A:160:VAL:HG23	2.15	0.61
1:D:175:LYS:HG2	1:D:180:GLU:HB2	1.82	0.61
1:D:341:ARG:CZ	1:D:405:VAL:HG11	2.29	0.61
1:C:54:ILE:HD11	1:D:133:LEU:HD23	1.81	0.61
1:C:343:LEU:HD21	1:C:409:GLU:HG2	1.83	0.61
1:D:319:HIS:O	1:D:322:HIS:NE2	2.34	0.61
1:D:383:ARG:O	1:D:383:ARG:HG2	1.99	0.60
1:A:216:LYS:HE3	1:A:217:TYR:CZ	2.36	0.60
1:A:131:VAL:HG21	1:A:172:LEU:HD11	1.82	0.60
1:B:264:ARG:NH1	1:B:281:LEU:O	2.35	0.60
1:C:290:THR:C	1:C:291:GLU:HG3	2.26	0.59
1:D:146:ASN:ND2	1:D:150:THR:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:GLY:HA2	3:D:502:ANP:H4'	1.84	0.59
1:D:319:HIS:O	1:D:322:HIS:CD2	2.56	0.59
1:D:278:PRO:HG2	1:D:282:PHE:H	1.68	0.59
1:B:305:LEU:HD11	1:B:358:ARG:HA	1.85	0.58
1:B:278:PRO:HD3	1:B:411:ILE:HD11	1.85	0.58
1:A:117:GLY:HA2	1:A:207:THR:OG1	2.02	0.58
1:B:414:ILE:O	1:B:418:ARG:HG2	2.04	0.58
1:D:278:PRO:HD3	1:D:411:ILE:HD11	1.86	0.58
1:B:202:LYS:HD2	1:B:202:LYS:H	1.68	0.58
1:C:346:ARG:HG2	1:C:346:ARG:NH1	2.17	0.58
1:D:193:LYS:NZ	1:D:194:LEU:HB3	2.18	0.58
1:A:343:LEU:HD11	1:A:409:GLU:HG2	1.86	0.57
1:A:145:ASN:ND2	1:A:147:ARG:HB2	2.19	0.57
1:B:399:LEU:O	1:B:403:GLN:HG3	2.04	0.57
1:D:341:ARG:NH2	1:D:405:VAL:HG11	2.19	0.57
1:C:319:HIS:O	1:C:322:HIS:CD2	2.57	0.57
1:B:126:GLU:HG2	1:B:133:LEU:HD13	1.85	0.57
1:C:88:VAL:HG21	1:C:235:LYS:HE3	1.87	0.56
1:A:99:ILE:HG12	1:A:242:LEU:HD11	1.87	0.56
1:A:327:ARG:HD3	1:A:356:TRP:CD2	2.40	0.56
1:C:79:LEU:HD22	1:C:163:VAL:HA	1.87	0.56
1:C:86:ASN:ND2	1:C:160:VAL:HG23	2.21	0.56
1:C:276:MET:CE	1:C:360:THR:CG2	2.83	0.56
1:B:319:HIS:O	1:B:322:HIS:HE1	1.89	0.55
1:D:341:ARG:HH22	1:D:405:VAL:HG21	1.71	0.55
1:D:337:PHE:CD1	1:D:401:LEU:HB3	2.41	0.55
1:B:276:MET:CE	1:B:281:LEU:HG	2.32	0.55
1:B:130:GLY:O	1:B:134:ILE:HG12	2.07	0.54
1:C:281:LEU:O	1:C:283:VAL:HG23	2.07	0.54
1:D:193:LYS:HG2	1:D:194:LEU:N	2.21	0.54
1:B:341:ARG:HH22	1:B:405:VAL:HG21	1.69	0.54
1:D:343:LEU:CD2	1:D:416:ILE:HD11	2.37	0.54
1:A:155:LEU:HD12	1:B:66:ARG:CD	2.36	0.54
1:A:233:ARG:NH2	1:A:270:GLU:OE2	2.40	0.54
1:A:108:SER:HB3	1:A:212:TRP:CD1	2.43	0.54
1:A:278:PRO:HG2	1:A:282:PHE:H	1.73	0.54
1:B:200:VAL:HG12	1:B:204:ASN:HB3	1.90	0.54
1:B:340:PHE:HE2	1:B:341:ARG:HE	1.55	0.54
1:C:311:VAL:HG21	1:C:380:LEU:HG	1.89	0.53
1:D:401:LEU:O	1:D:405:VAL:HA	2.07	0.53
1:A:61:ASP:O	1:A:65:ARG:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:GLN:HG3	1:C:243:THR:HB	1.91	0.53
1:B:183:MET:HE3	1:B:185:PHE:CZ	2.43	0.53
1:B:268:LYS:HG3	1:B:281:LEU:HD12	1.91	0.53
1:D:126:GLU:OE2	1:D:137:ARG:NH2	2.38	0.53
1:B:79:LEU:HG	1:B:163:VAL:HA	1.91	0.53
1:D:345:PRO:O	1:D:348:VAL:HG22	2.09	0.52
1:A:155:LEU:HD12	1:B:66:ARG:CZ	2.34	0.52
1:C:274:HIS:CE1	1:C:302:GLU:OE1	2.62	0.52
1:D:314:ILE:HD11	1:D:372:PHE:CE1	2.44	0.52
1:A:124:PRO:C	1:A:125:GLU:HG3	2.34	0.52
1:C:101:VAL:HG22	1:C:111:VAL:HG22	1.91	0.52
1:B:48:ARG:HG3	1:B:49:TYR:N	2.25	0.52
1:D:126:GLU:O	1:D:127:LYS:HB2	2.09	0.52
1:A:311:VAL:HG21	1:A:380:LEU:HG	1.92	0.52
1:D:338:CYS:SG	1:D:343:LEU:HD22	2.49	0.52
1:C:104:TYR:HA	1:C:249:GLU:HG2	1.91	0.51
1:C:274:HIS:ND1	1:C:302:GLU:OE1	2.43	0.51
1:A:123:HIS:ND1	1:A:126:GLU:HB2	2.25	0.51
1:A:319:HIS:O	1:A:322:HIS:CD2	2.63	0.51
1:A:281:LEU:O	1:A:283:VAL:HG23	2.10	0.51
1:A:331:THR:HG22	1:A:335:ARG:NE	2.25	0.51
1:D:378:GLU:HA	1:D:378:GLU:OE2	2.10	0.51
1:D:322:HIS:HB2	1:D:389:ILE:HD12	1.92	0.51
1:D:365:LEU:HD13	1:D:389:ILE:HD11	1.93	0.51
1:C:145:ASN:CG	1:C:147:ARG:H	2.19	0.51
1:A:268:LYS:HG3	1:A:281:LEU:HD12	1.93	0.50
1:B:248:ASP:HB3	1:B:251:THR:OG1	2.11	0.50
1:A:229:ARG:NH2	1:A:253:GLU:OE1	2.43	0.50
1:D:399:LEU:O	1:D:403:GLN:CG	2.56	0.50
1:D:401:LEU:HD22	1:D:408:GLY:HA3	1.94	0.50
1:D:338:CYS:O	1:D:343:LEU:N	2.44	0.50
1:B:200:VAL:CG1	1:B:204:ASN:HB3	2.42	0.50
1:D:341:ARG:NH1	1:D:405:VAL:HG11	2.27	0.49
1:D:353:GLU:O	1:D:357:ASP:N	2.45	0.49
1:A:328:SER:HB2	1:A:390:GLU:HG3	1.94	0.49
1:D:343:LEU:HD23	1:D:343:LEU:O	2.12	0.49
1:A:251:THR:HA	1:D:383:ARG:HH12	1.77	0.49
1:B:327:ARG:HG3	1:B:356:TRP:CD2	2.48	0.49
1:C:278:PRO:HD3	1:C:411:ILE:HD11	1.95	0.49
1:C:141:GLY:HA2	3:C:502:ANP:H4'	1.94	0.49
1:D:373:SER:OG	1:D:379:ARG:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:HD22	1:A:359:VAL:O	2.12	0.49
1:D:349:LYS:HB2	1:D:349:LYS:HE3	1.58	0.49
1:D:193:LYS:CG	1:D:194:LEU:H	2.21	0.49
1:D:291:GLU:HB3	1:D:388:PHE:CE2	2.47	0.49
1:A:86:ASN:HD22	1:A:160:VAL:HG23	1.78	0.48
1:A:365:LEU:HD21	1:A:367:MET:HE2	1.95	0.48
1:B:216:LYS:HE2	1:B:217:TYR:CZ	2.49	0.48
1:C:365:LEU:HD13	1:C:389:ILE:HD11	1.95	0.48
1:A:273:GLU:HG2	1:A:274:HIS:N	2.27	0.48
3:C:502:ANP:O2'	1:D:49:TYR:OH	2.16	0.48
1:D:102:THR:HG23	1:D:247:HIS:HB3	1.94	0.48
1:A:367:MET:HE1	1:A:385:ALA:HB2	1.95	0.48
1:C:367:MET:HE1	1:C:385:ALA:HB2	1.96	0.48
1:D:327:ARG:CD	1:D:352:PRO:HB3	2.40	0.48
1:B:128:ILE:HD12	1:B:132:GLU:HG2	1.96	0.48
1:C:360:THR:HG23	1:C:360:THR:O	2.14	0.48
1:C:291:GLU:HA	1:C:366:LYS:O	2.14	0.48
1:A:407:ILE:O	1:A:411:ILE:HG13	2.14	0.48
1:C:102:THR:HG23	1:C:247:HIS:HB3	1.96	0.48
1:C:318:GLN:OE1	1:D:318:GLN:NE2	2.32	0.48
1:D:145:ASN:OD1	1:D:147:ARG:HB2	2.14	0.48
1:A:126:GLU:HG2	1:A:133:LEU:HD13	1.96	0.47
1:A:300:VAL:HG22	1:A:305:LEU:HD21	1.96	0.47
1:B:48:ARG:CG	1:B:49:TYR:N	2.78	0.47
1:D:117:GLY:HA2	1:D:207:THR:OG1	2.14	0.47
1:A:86:ASN:HB3	3:A:502:ANP:N7	2.29	0.47
1:B:103:LEU:HD11	1:B:228:LEU:HD23	1.96	0.47
1:C:210:ARG:HG2	1:C:212:TRP:CH2	2.50	0.47
1:D:324:ASN:HD22	1:D:327:ARG:HH12	1.61	0.47
1:D:341:ARG:NH2	1:D:405:VAL:CG1	2.77	0.47
1:A:239:CYS:HB2	1:A:313:LEU:HD21	1.96	0.47
1:B:225:VAL:HG21	1:B:248:ASP:OD1	2.15	0.47
1:B:291:GLU:HA	1:B:366:LYS:O	2.14	0.47
1:B:417:ASP:O	1:B:420:SER:HB2	2.15	0.47
1:D:341:ARG:CZ	1:D:405:VAL:CG1	2.92	0.47
1:B:277:LEU:HD23	1:B:411:ILE:HG12	1.98	0.46
1:D:286:LEU:HD22	1:D:392:ALA:HB2	1.97	0.46
1:B:99:ILE:HG12	1:B:242:LEU:HD11	1.96	0.46
1:B:284:GLY:HA3	1:B:295:TRP:CZ2	2.49	0.46
1:A:369:ASP:HA	1:B:66:ARG:HH22	1.81	0.46
1:B:365:LEU:HD21	1:B:367:MET:HE2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:LYS:HG2	1:D:180:GLU:CB	2.46	0.46
1:B:122:ILE:CD1	1:B:122:ILE:CB	2.79	0.46
1:B:367:MET:HE3	1:B:370:PRO:HB3	1.97	0.46
1:C:350:LEU:HD11	1:C:415:ALA:HB1	1.98	0.46
1:D:276:MET:HB2	1:D:276:MET:HE3	1.56	0.46
1:A:341:ARG:NH1	1:A:409:GLU:OE1	2.48	0.46
1:B:98:GLN:HA	1:B:243:THR:O	2.15	0.46
1:C:288:LYS:C	1:C:290:THR:H	2.22	0.46
1:C:328:SER:OG	1:C:390:GLU:HG3	2.16	0.46
1:C:135:LEU:HD22	1:C:160:VAL:HG11	1.99	0.45
1:C:327:ARG:HG3	1:C:356:TRP:CE3	2.50	0.45
1:B:86:ASN:HD21	1:B:160:VAL:HG23	1.80	0.45
1:D:334:LEU:HD23	1:D:350:LEU:HD13	1.98	0.45
1:C:134:ILE:HD12	3:C:502:ANP:H4'	1.99	0.45
1:B:276:MET:HG2	1:B:300:VAL:HG22	1.98	0.45
1:A:300:VAL:CG2	1:A:305:LEU:HD21	2.46	0.45
1:A:156:HIS:CD2	1:B:66:ARG:HD3	2.52	0.45
1:C:130:GLY:O	1:C:134:ILE:HG12	2.17	0.45
1:C:251:THR:HG23	1:C:253:GLU:HB2	1.99	0.45
1:C:322:HIS:CD2	1:C:322:HIS:H	2.34	0.45
1:A:277:LEU:HD23	1:A:411:ILE:HG12	1.98	0.45
1:B:341:ARG:CZ	1:B:405:VAL:HG21	2.44	0.45
1:C:321:THR:OG1	1:C:382:SER:O	2.25	0.45
1:D:176:ARG:CD	1:D:177:GLU:OE1	2.65	0.45
1:A:273:GLU:CD	1:A:273:GLU:H	2.23	0.44
1:D:401:LEU:HD23	1:D:401:LEU:HA	1.72	0.44
1:C:327:ARG:NH1	1:C:352:PRO:HB2	2.33	0.44
1:D:345:PRO:HG2	1:D:348:VAL:HG11	2.00	0.44
1:A:66:ARG:NH1	4:A:604:HOH:O	2.32	0.44
1:A:288:LYS:C	1:A:290:THR:H	2.25	0.44
1:C:291:GLU:HG2	1:C:367:MET:HB2	2.00	0.44
1:D:177:GLU:OE1	1:D:177:GLU:N	2.51	0.44
1:B:277:LEU:HD21	1:B:410:LYS:HB2	1.99	0.44
1:C:170:VAL:HG22	1:C:211:PHE:CB	2.47	0.44
1:C:216:LYS:HE3	1:C:217:TYR:CZ	2.53	0.44
1:A:300:VAL:HG23	1:A:358:ARG:NH2	2.32	0.44
1:B:60:LEU:HD13	1:B:165:ALA:HB2	1.99	0.44
1:B:278:PRO:HG2	1:B:282:PHE:H	1.81	0.44
1:C:327:ARG:HA	1:C:356:TRP:CZ3	2.53	0.44
1:B:134:ILE:HG23	3:B:502:ANP:H5'1	2.00	0.44
1:C:95:HIS:CE1	1:C:116:ARG:HD3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:ARG:NH2	1:C:270:GLU:OE2	2.51	0.43
1:A:273:GLU:HG3	1:A:274:HIS:CE1	2.54	0.43
1:B:135:LEU:HD22	1:B:160:VAL:HG11	2.01	0.43
1:C:99:ILE:HA	1:C:112:SER:O	2.18	0.43
1:D:193:LYS:CG	1:D:194:LEU:N	2.81	0.43
1:A:343:LEU:CD1	1:A:409:GLU:HG2	2.47	0.43
1:B:267:LEU:HB3	1:B:281:LEU:HD11	2.01	0.43
1:C:98:GLN:HA	1:C:243:THR:O	2.19	0.43
1:A:141:GLY:HA2	3:A:502:ANP:H4'	1.99	0.43
1:C:86:ASN:HD21	1:C:160:VAL:HG23	1.84	0.43
1:D:311:VAL:O	1:D:314:ILE:HG13	2.19	0.43
1:A:319:HIS:O	1:A:322:HIS:NE2	2.52	0.43
1:B:124:PRO:C	1:B:125:GLU:CG	2.87	0.43
1:D:89:ASP:CG	1:D:153:GLY:H	2.21	0.43
1:A:365:LEU:HD21	1:A:367:MET:CE	2.49	0.43
1:C:233:ARG:HB2	1:C:257:TRP:CE2	2.53	0.43
1:C:290:THR:C	1:C:291:GLU:CG	2.92	0.43
1:D:146:ASN:HB3	1:D:150:THR:HA	2.01	0.43
1:D:412:ALA:C	1:D:416:ILE:HD12	2.44	0.43
1:B:278:PRO:HB3	1:B:407:ILE:HG21	2.00	0.42
1:C:108:SER:HB2	1:C:212:TRP:CD1	2.54	0.42
1:B:248:ASP:HB3	1:B:251:THR:HG1	1.83	0.42
1:B:267:LEU:HD13	1:B:362:VAL:HG23	2.01	0.42
1:D:320:GLY:HA3	1:D:380:LEU:H	1.84	0.42
1:A:367:MET:CE	1:A:385:ALA:HB2	2.50	0.42
1:B:200:VAL:HG12	1:B:201:GLY:N	2.34	0.42
1:D:341:ARG:HH22	1:D:405:VAL:HG11	1.84	0.42
1:B:300:VAL:O	1:B:358:ARG:NH1	2.53	0.42
1:A:363:LEU:HD11	1:A:389:ILE:HD13	2.02	0.42
1:C:155:LEU:HD21	1:C:372:PHE:HD2	1.85	0.42
1:C:356:TRP:HA	1:C:359:VAL:HG23	2.00	0.42
1:C:155:LEU:HD21	1:C:372:PHE:CD2	2.54	0.42
1:C:215:PRO:HB3	1:C:221:PRO:HG3	2.01	0.42
1:A:116:ARG:NH1	1:B:49:TYR:HB2	2.35	0.42
1:A:156:HIS:HD2	1:B:66:ARG:HD3	1.85	0.42
1:C:176:ARG:NH2	1:D:49:TYR:O	2.52	0.42
1:D:126:GLU:CD	1:D:137:ARG:NH2	2.73	0.42
1:D:278:PRO:CG	1:D:282:PHE:H	2.31	0.41
1:B:319:HIS:HB3	1:B:323:VAL:HG21	2.03	0.41
1:C:113:ASP:OD2	1:C:207:THR:N	2.44	0.41
1:A:100:GLU:HG3	1:A:245:LYS:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:TYR:HE1	1:C:110:GLU:HB3	1.85	0.41
1:D:118:MET:HB2	1:D:174:ILE:HD13	2.01	0.41
1:A:126:GLU:HG3	1:A:137:ARG:NH2	2.35	0.41
1:D:331:THR:HG22	1:D:355:VAL:HB	2.02	0.41
1:B:344:LEU:HD12	1:B:348:VAL:HG13	2.03	0.41
1:C:48:ARG:HH11	1:C:48:ARG:HG2	1.85	0.41
1:D:176:ARG:CG	1:D:177:GLU:OE1	2.66	0.41
1:A:287:LYS:HE3	1:A:289:ASP:OD2	2.21	0.41
1:B:108:SER:HB3	1:B:212:TRP:CD1	2.55	0.41
1:B:142:GLY:H	3:B:502:ANP:HO3'	1.66	0.41
1:C:74:ALA:HA	1:C:219:ASP:OD2	2.21	0.41
1:D:99:ILE:HA	1:D:112:SER:O	2.21	0.41
1:D:235:LYS:NZ	1:D:313:LEU:O	2.38	0.41
1:C:356:TRP:HA	1:C:359:VAL:CG2	2.51	0.41
1:D:246:LEU:HB3	1:D:255:ASP:HB2	2.03	0.41
1:D:286:LEU:HB3	1:D:293:VAL:HG12	2.03	0.40
1:D:337:PHE:HE1	1:D:402:ASN:HD22	1.70	0.40
1:A:54:ILE:HD12	1:B:134:ILE:HD11	2.03	0.40
1:D:343:LEU:CD2	1:D:416:ILE:CD1	2.94	0.40
1:B:121:ASP:OD1	1:B:121:ASP:N	2.53	0.40
1:B:129:PRO:HD2	1:B:132:GLU:OE2	2.22	0.40
1:B:311:VAL:HG21	1:B:380:LEU:HG	2.03	0.40
3:D:502:ANP:O1A	3:D:502:ANP:O2B	2.39	0.40
1:D:176:ARG:NH1	1:D:177:GLU:OE2	2.54	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	372/408 (91%)	354 (95%)	18 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	372/408 (91%)	355 (95%)	17 (5%)	0	100	100
1	C	372/408 (91%)	354 (95%)	18 (5%)	0	100	100
1	D	372/408 (91%)	352 (95%)	20 (5%)	0	100	100
All	All	1488/1632 (91%)	1415 (95%)	73 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	309/340 (91%)	309 (100%)	0	100	100
1	B	309/340 (91%)	307 (99%)	2 (1%)	78	92
1	C	309/340 (91%)	308 (100%)	1 (0%)	86	95
1	D	309/340 (91%)	309 (100%)	0	100	100
All	All	1236/1360 (91%)	1233 (100%)	3 (0%)	87	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	143	LYS
1	B	380	LEU
1	C	102	THR

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

Mol	Chain	Res	Type
1	A	146	ASN
1	A	156	HIS
1	A	322	HIS
1	A	324	ASN
1	A	371	GLN

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Mol	Chain	Res	Type
1	B	78	HIS
1	B	164	ASN
1	B	274	HIS
1	B	402	ASN
1	C	375	GLN
1	C	394	HIS
1	D	50	ASN
1	D	274	HIS
1	D	402	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	ANP	C	502	2	33,33,33	0.94	4 (12%)	45,52,52	0.74	0
3	ANP	B	502	2	33,33,33	1.03	4 (12%)	45,52,52	0.68	2 (4%)
3	ANP	D	502	2	33,33,33	0.93	4 (12%)	45,52,52	0.85	1 (2%)
3	ANP	A	502	2	33,33,33	1.00	4 (12%)	45,52,52	0.81	0

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	ANP	C	502	2	-	4/18/38/38	0/3/3/3
3	ANP	B	502	2	-	3/18/38/38	0/3/3/3
3	ANP	D	502	2	-	4/18/38/38	0/3/3/3
3	ANP	A	502	2	-	2/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ANP	PG-N3B	2.94	1.71	1.63
3	B	502	ANP	PG-O1G	2.67	1.50	1.46
3	B	502	ANP	PB-O1B	2.65	1.50	1.46
3	A	502	ANP	PG-O1G	2.55	1.50	1.46
3	C	502	ANP	PG-O1G	2.53	1.50	1.46
3	A	502	ANP	PG-N3B	2.49	1.69	1.63
3	C	502	ANP	PG-N3B	2.46	1.69	1.63
3	A	502	ANP	PB-O1B	2.45	1.49	1.46
3	D	502	ANP	PG-O1G	2.41	1.49	1.46
3	C	502	ANP	PB-O1B	2.39	1.49	1.46
3	D	502	ANP	PB-O1B	2.38	1.49	1.46
3	B	502	ANP	PB-O3A	-2.37	1.56	1.59
3	A	502	ANP	PB-O3A	-2.34	1.56	1.59
3	D	502	ANP	PG-N3B	2.28	1.69	1.63
3	D	502	ANP	PB-O3A	-2.17	1.56	1.59
3	C	502	ANP	PB-O3A	-2.03	1.56	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	502	ANP	O1B-PB-N3B	-2.61	107.92	111.77
3	B	502	ANP	O2B-PB-O3A	2.39	112.62	104.64
3	B	502	ANP	O1B-PB-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	ANP	PB-N3B-PG-O1G

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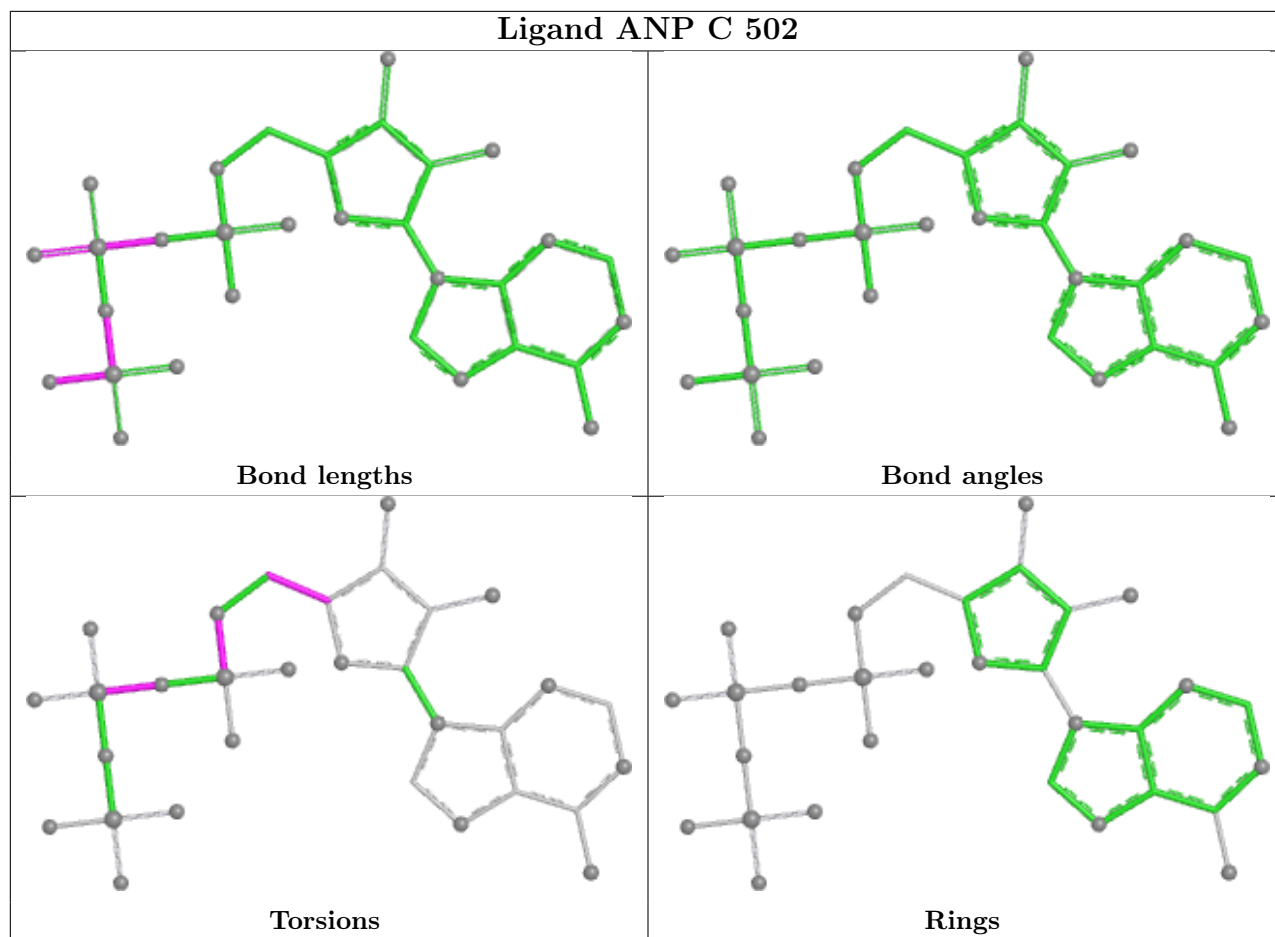
Mol	Chain	Res	Type	Atoms
3	B	502	ANP	PB-N3B-PG-O1G
3	B	502	ANP	PG-N3B-PB-O1B
3	B	502	ANP	PB-O3A-PA-O5'
3	C	502	ANP	PA-O3A-PB-O2B
3	D	502	ANP	O4'-C4'-C5'-O5'
3	C	502	ANP	O4'-C4'-C5'-O5'
3	C	502	ANP	C3'-C4'-C5'-O5'
3	D	502	ANP	C3'-C4'-C5'-O5'
3	C	502	ANP	C5'-O5'-PA-O3A
3	D	502	ANP	C5'-O5'-PA-O3A
3	A	502	ANP	PA-O3A-PB-O2B
3	D	502	ANP	PB-N3B-PG-O1G

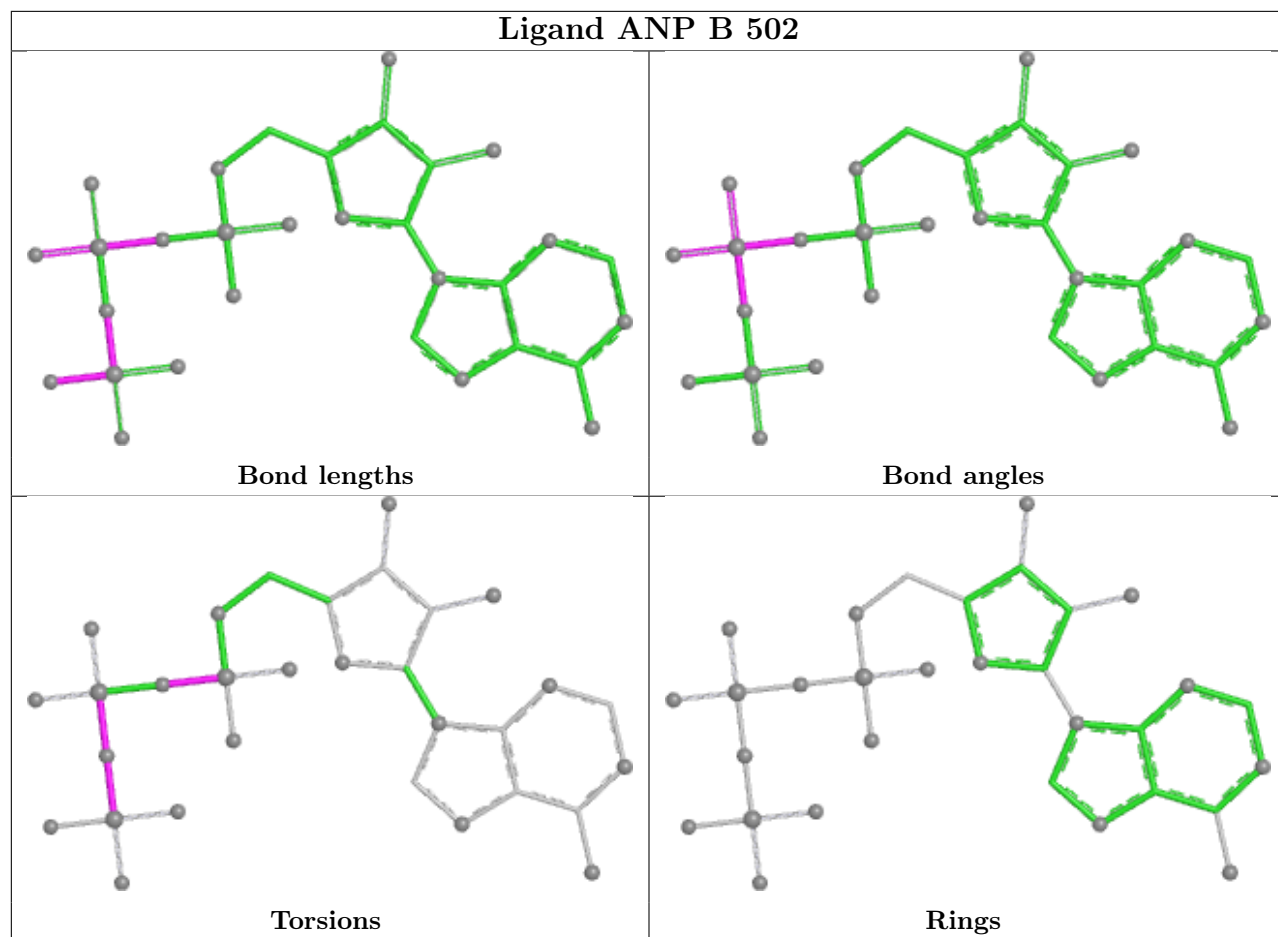
There are no ring outliers.

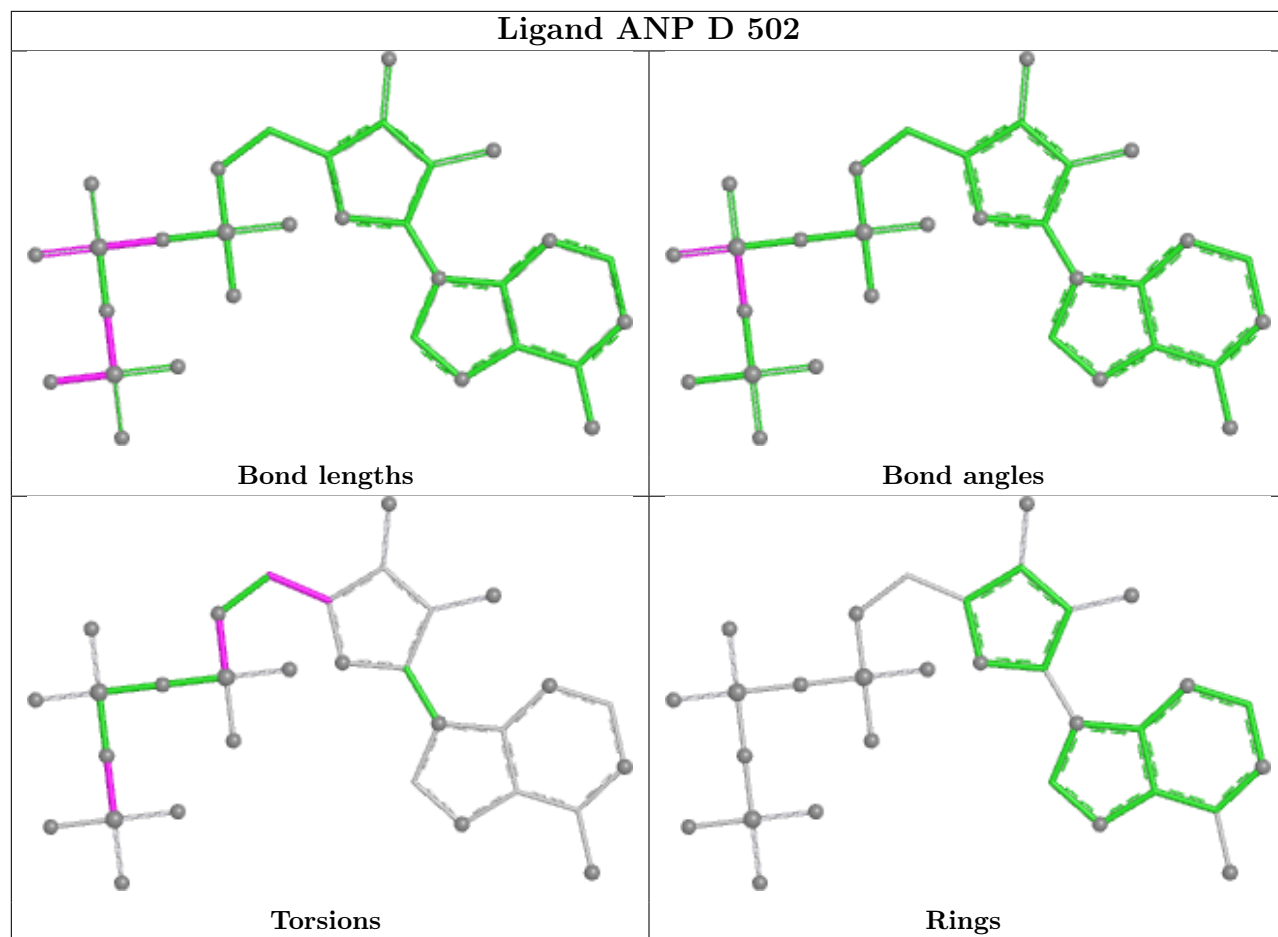
4 monomers are involved in 9 short contacts:

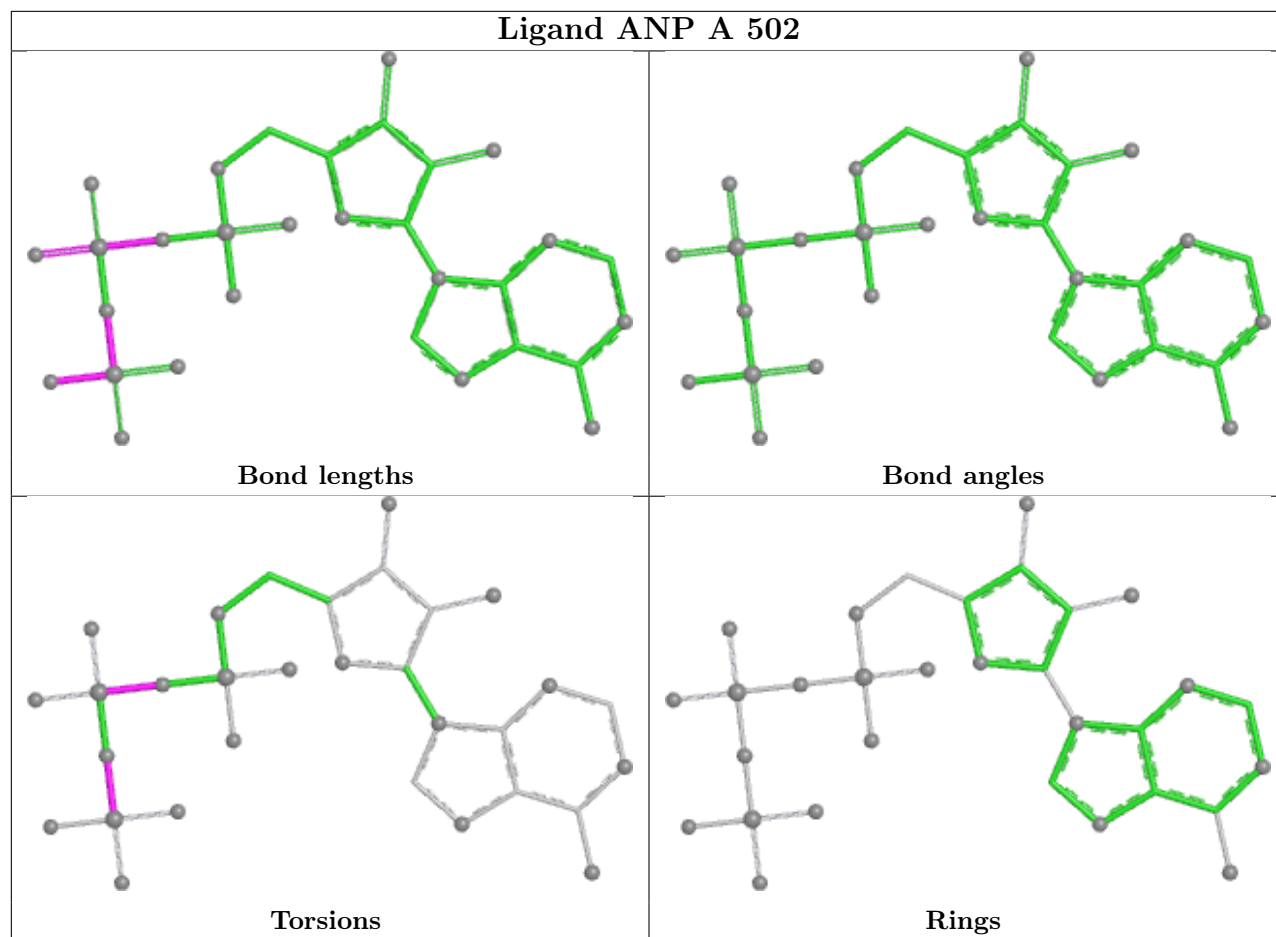
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	ANP	3	0
3	B	502	ANP	2	0
3	D	502	ANP	2	0
3	A	502	ANP	2	0

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.









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	374/408 (91%)	0.03	6 (1%) 70 63	29, 46, 78, 118	0
1	B	374/408 (91%)	0.15	7 (1%) 66 58	24, 50, 88, 100	0
1	C	374/408 (91%)	0.07	8 (2%) 63 55	25, 48, 92, 118	0
1	D	374/408 (91%)	0.09	9 (2%) 59 50	27, 51, 83, 119	0
All	All	1496/1632 (91%)	0.08	30 (2%) 65 57	24, 48, 87, 119	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	340	PHE	4.1
1	D	343	LEU	3.6
1	B	48	ARG	3.0
1	D	339	ASP	2.6
1	C	226	ARG	2.6
1	C	421	ALA	2.5
1	C	145	ASN	2.5
1	B	342	ASN	2.5
1	D	147	ARG	2.4
1	A	345	PRO	2.4
1	A	421	ALA	2.4
1	C	289	ASP	2.3
1	B	421	ALA	2.3
1	D	340	PHE	2.3
1	A	277	LEU	2.3
1	B	66	ARG	2.3
1	B	281	LEU	2.3
1	B	409	GLU	2.2
1	B	343	LEU	2.2
1	D	273	GLU	2.2
1	C	254	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	48	ARG	2.2
1	D	341	ARG	2.2
1	A	406	GLU	2.2
1	A	50	ASN	2.2
1	C	408	GLY	2.1
1	D	289	ASP	2.1
1	D	353	GLU	2.1
1	D	402	ASN	2.0
1	C	48	ARG	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 [\(i\)](#)

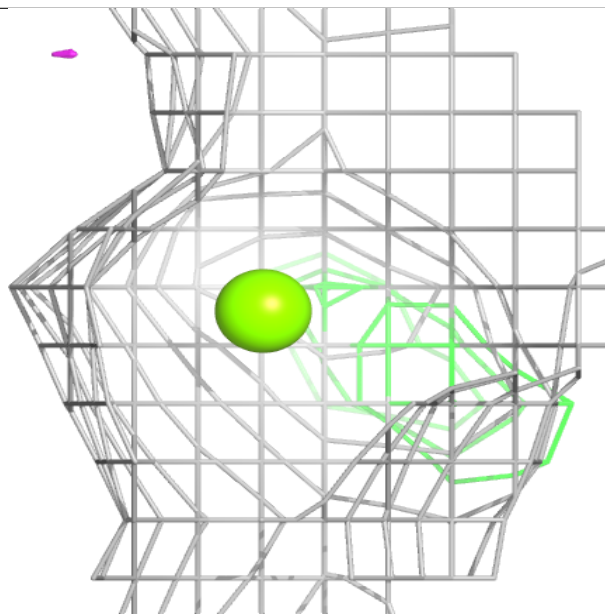
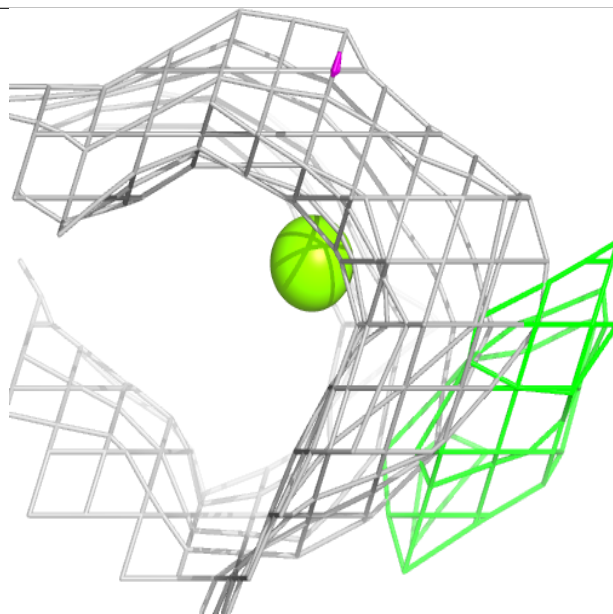
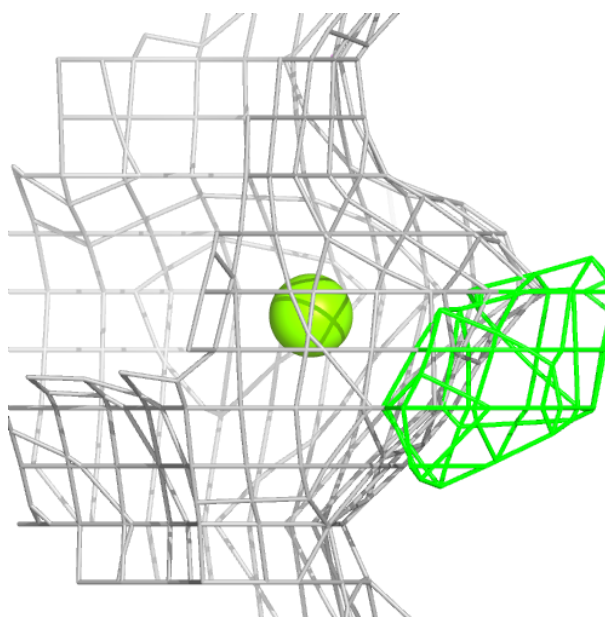
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	C	501	1/1	0.88	0.11	40,40,40,40	0
2	MG	B	501	1/1	0.92	0.13	37,37,37,37	0
3	ANP	C	502	31/31	0.95	0.08	27,33,41,42	0
3	ANP	D	502	31/31	0.95	0.09	32,44,53,56	0
3	ANP	A	502	31/31	0.96	0.08	27,40,48,50	0
3	ANP	B	502	31/31	0.96	0.07	29,34,43,45	0
2	MG	A	501	1/1	0.97	0.04	27,27,27,27	0
2	MG	D	501	1/1	0.97	0.07	44,44,44,44	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.

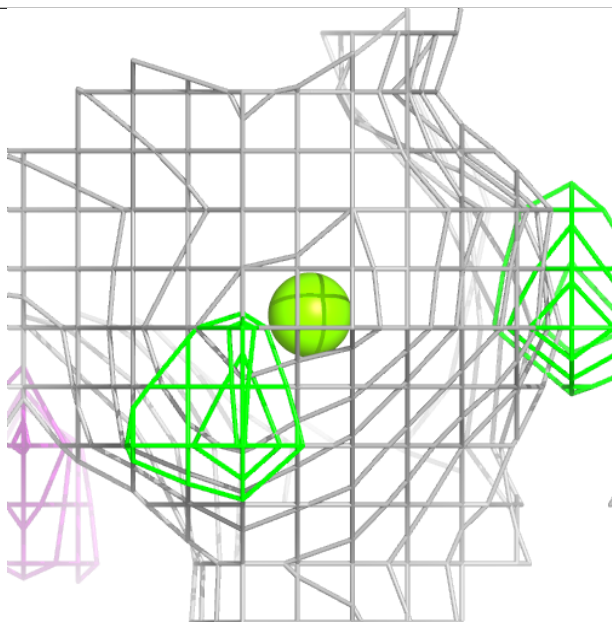
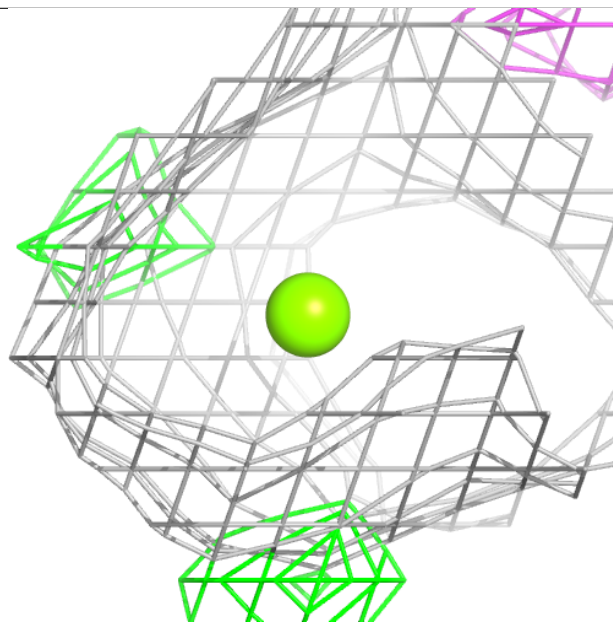
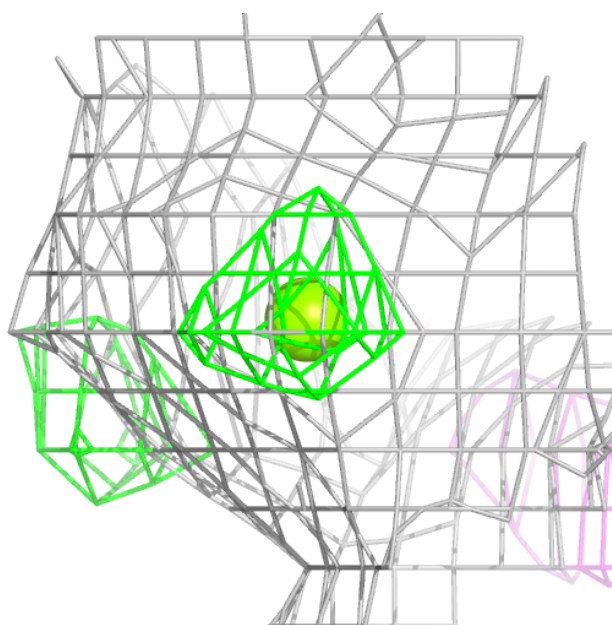
Electron density around MG C 501:

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



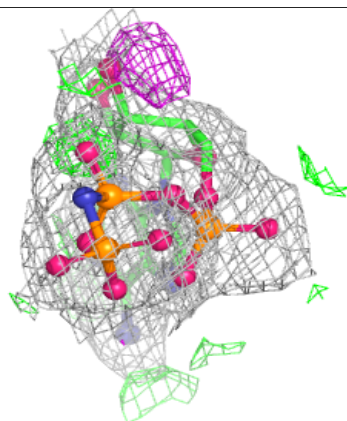
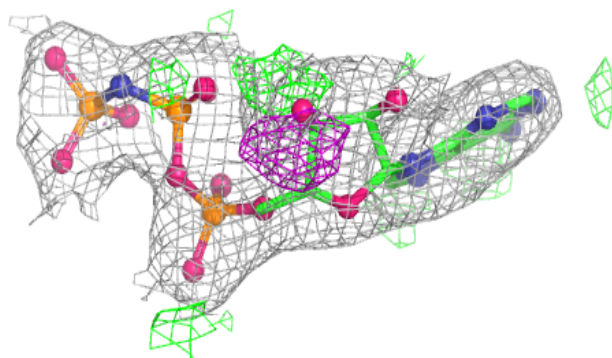
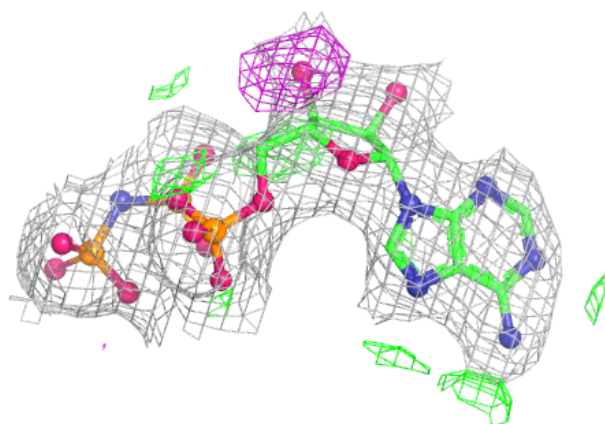
Electron density around MG B 501:

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

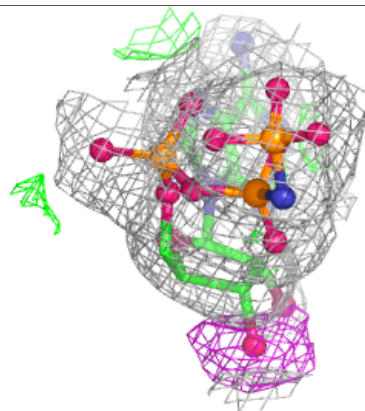
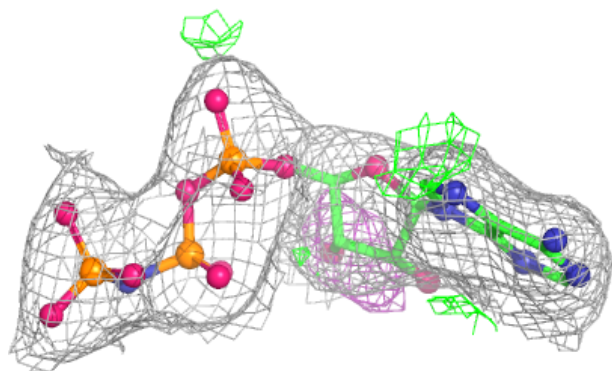
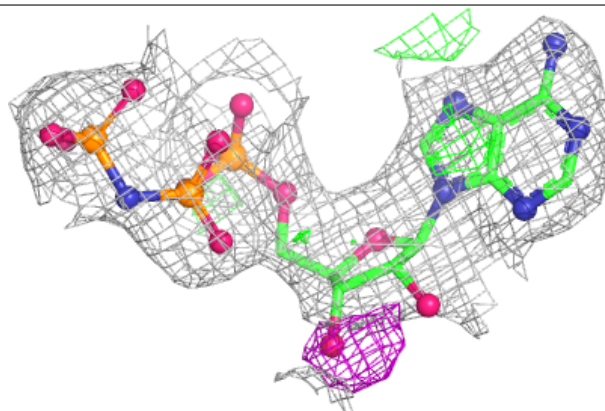


Electron density around ANP C 502:

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

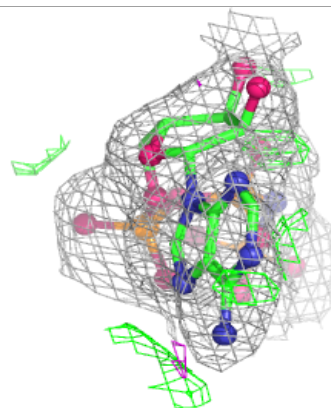
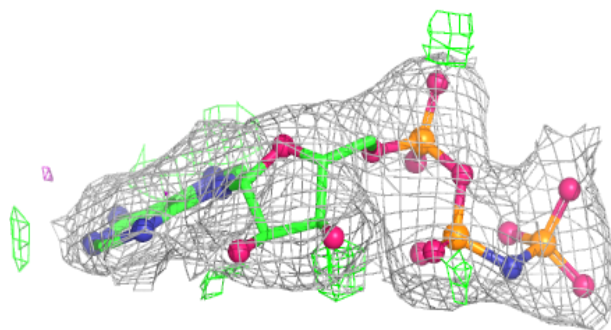
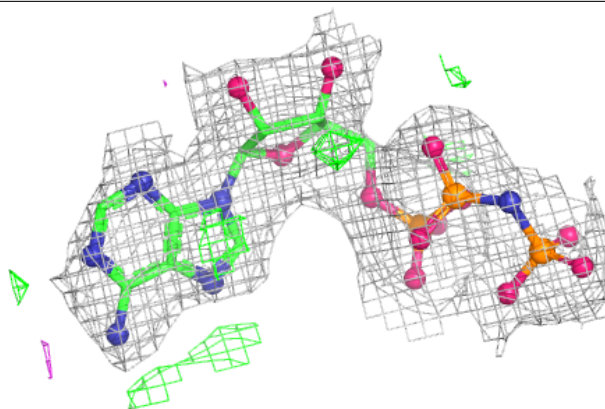
**Electron density around ANP D 502:**

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

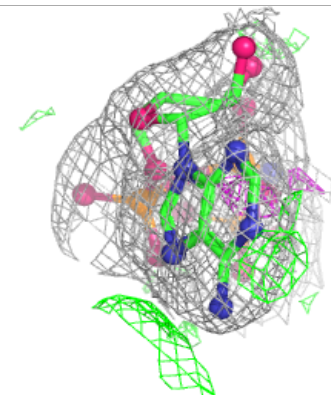
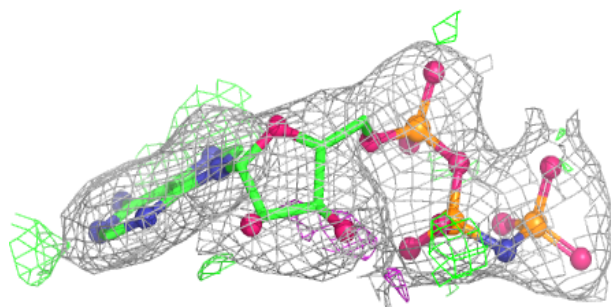
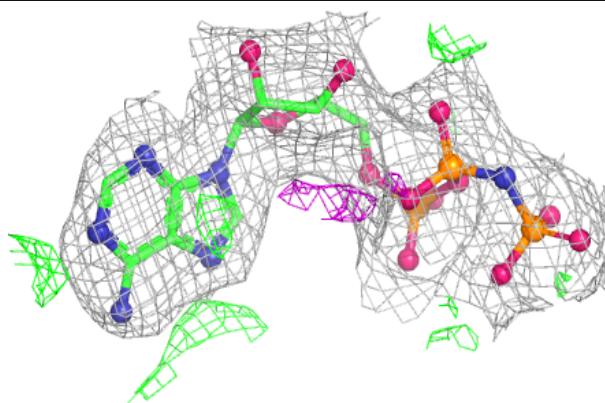


Electron density around ANP A 502:

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

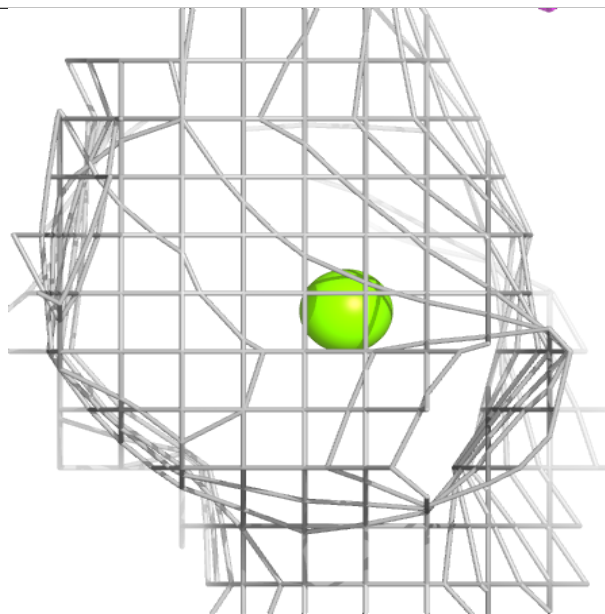
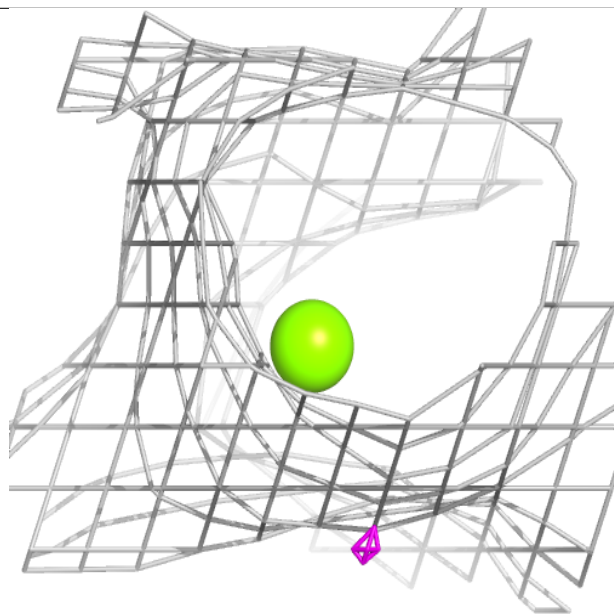
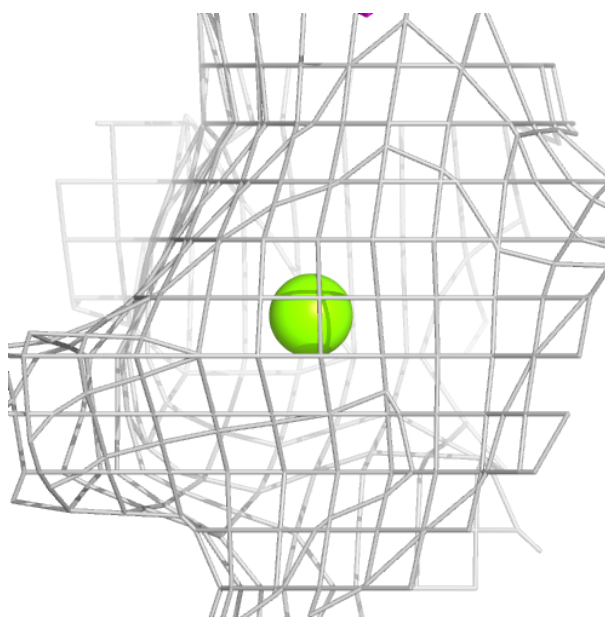
**Electron density around ANP B 502:**

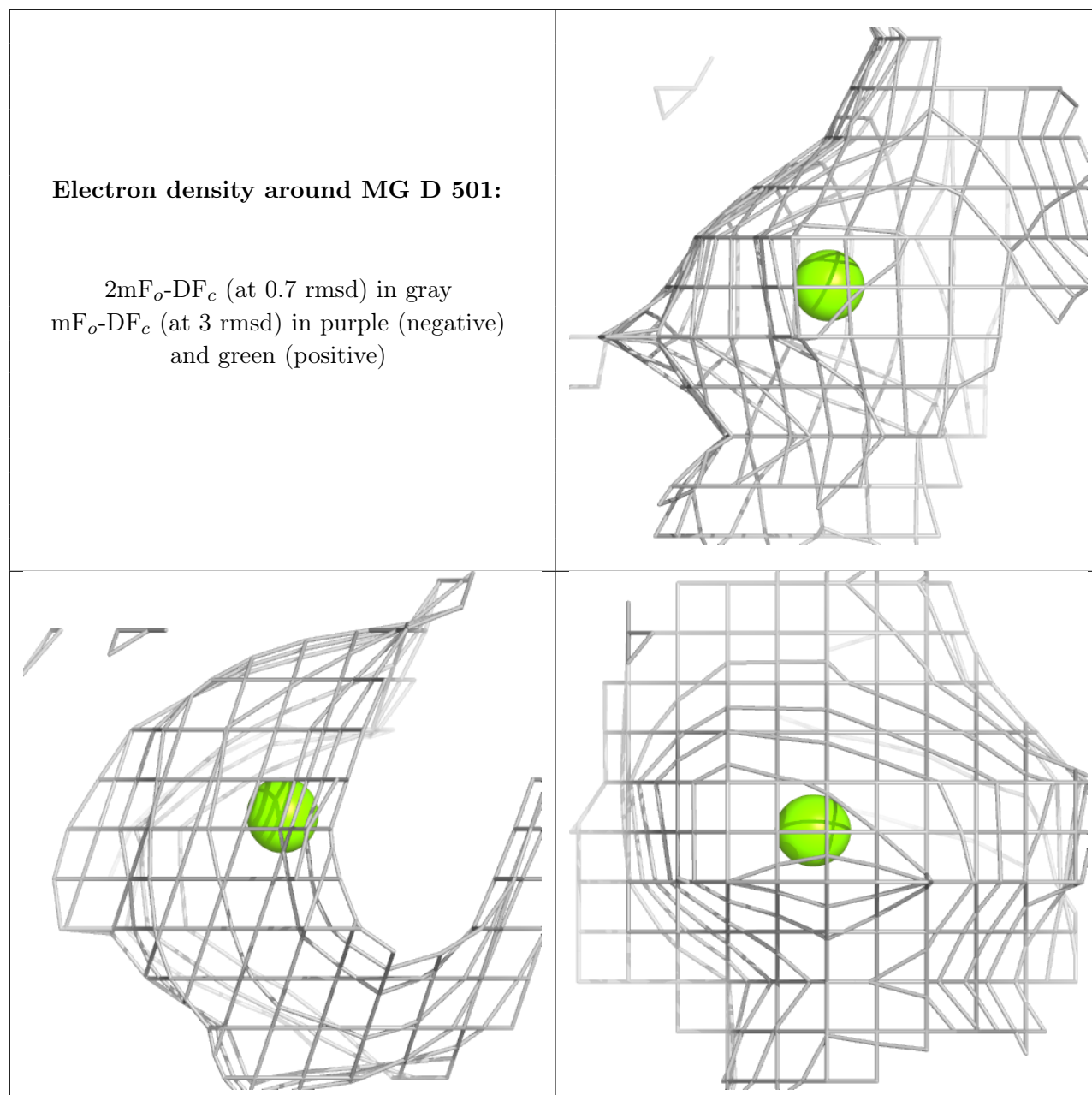
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 501:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.