



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:22 PM UTC

PDB ID : 7RSM / pdb_00007rsm
Title : Crystal structure of pyrrolysyl-tRNA synthetase (N346D/C348S/Y384F) in complex with o-Chlorophenylalanine and AMP-PNP
Authors : Yang, K.; Liu, W.
Deposited on : 2021-08-11
Resolution : 2.15 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

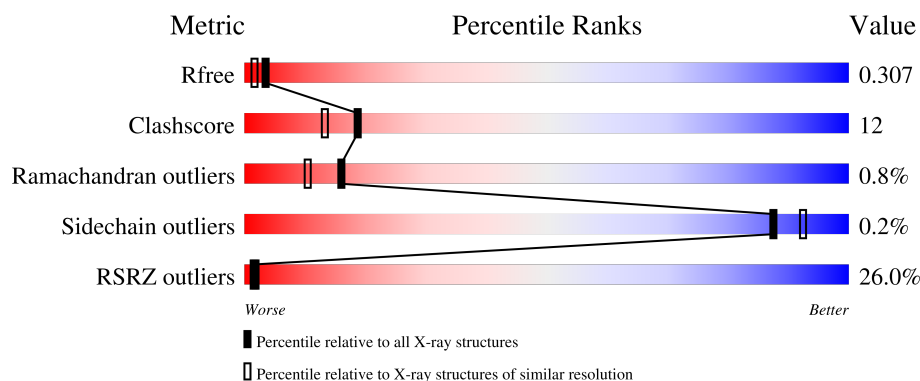
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	267	19% 82% 17% .
1	B	267	23% 72% 27% .
1	C	267	28% 75% 24% .
1	D	267	34% 78% 20% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	2L5	A	502	-	-	X	-
3	2L5	B	502	-	-	X	-
3	2L5	D	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9181 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 Pyrrolysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	0	0
			2168	1379	370	409	10			
1	B	267	Total	C	N	O	S	0	0	0
			2168	1379	370	409	10			
1	C	267	Total	C	N	O	S	0	0	0
			2168	1379	370	409	10			
1	D	267	Total	C	N	O	S	0	0	0
			2168	1379	370	409	10			

There are 12 discrepancies between the modelled and reference sequences:

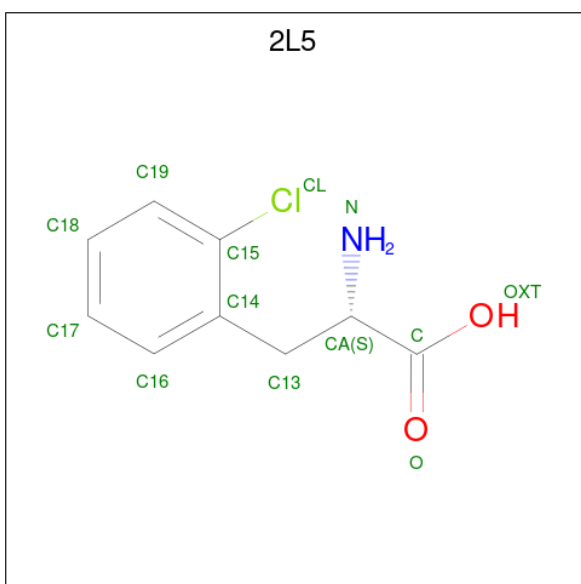
Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
A	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
A	384	PHE	TYR	engineered mutation	UNP A0A0F8JXW8
B	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
B	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
B	384	PHE	TYR	engineered mutation	UNP A0A0F8JXW8
C	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
C	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
C	384	PHE	TYR	engineered mutation	UNP A0A0F8JXW8
D	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
D	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
D	384	PHE	TYR	engineered mutation	UNP A0A0F8JXW8

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	B	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	C	1	Total 31	C 10	N 6	O 12	P 3	0	0
2	D	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 3 is 2-chloro-L-phenylalanine (CCD ID: 2L5) (formula: $\text{C}_9\text{H}_{10}\text{ClNO}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 13	C 9	Cl 1	N 1	O 2	0	0
3	B	1	Total 13	C 9	Cl 1	N 1	O 2	0	0
3	C	1	Total 13	C 9	Cl 1	N 1	O 2	0	0
3	D	1	Total 13	C 9	Cl 1	N 1	O 2	0	0

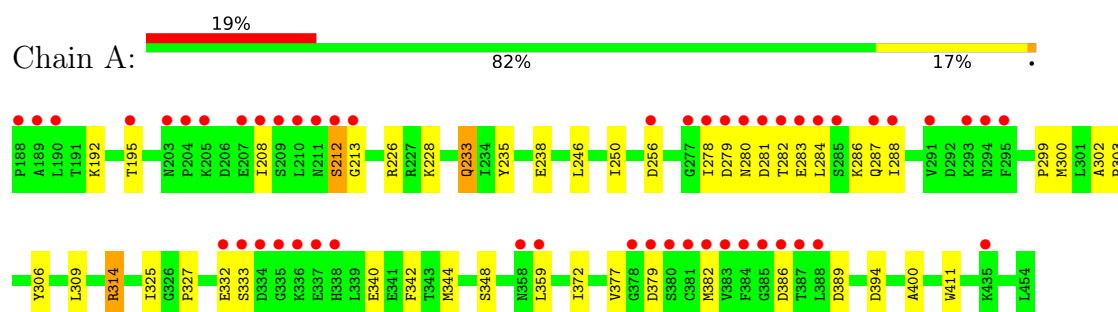
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total 100	O 100	0	0
4	B	89	Total 89	O 89	0	0
4	C	61	Total 61	O 61	0	0
4	D	83	Total 83	O 83	0	0

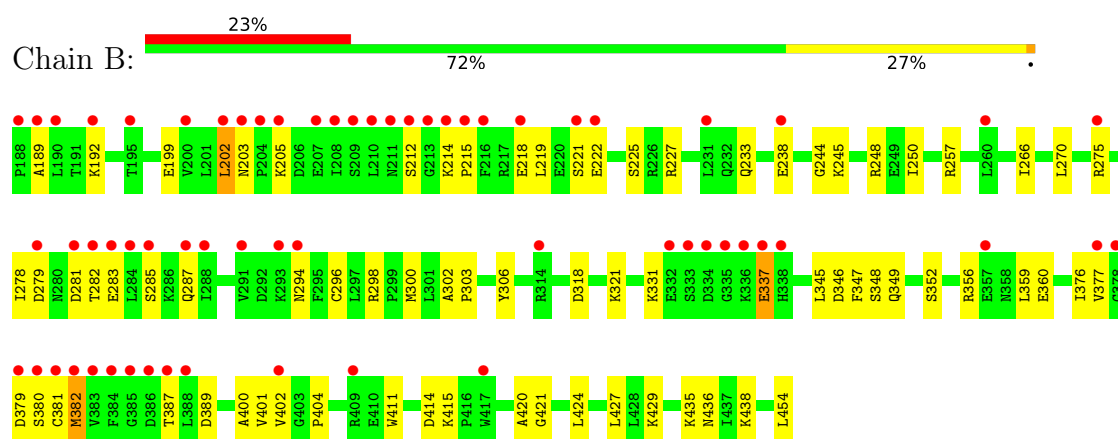
3 Residue-property plots [i](#)

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.

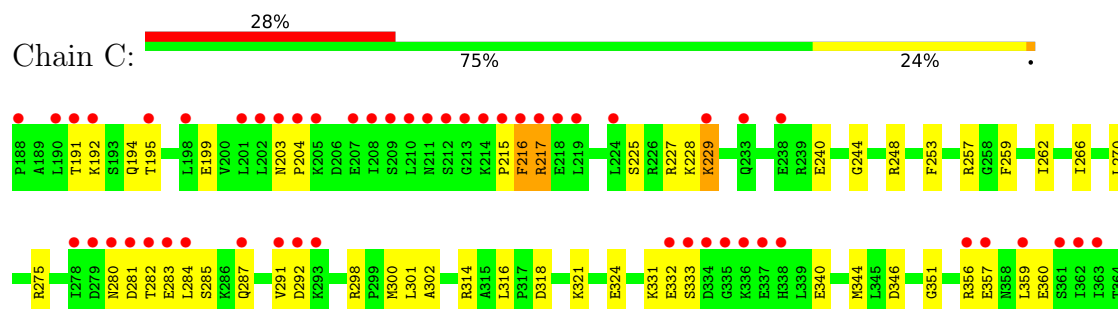
• Molecule 1: Pyrrolysine-tRNA ligase



• Molecule 1: Pyrrolysine-tRNA ligase

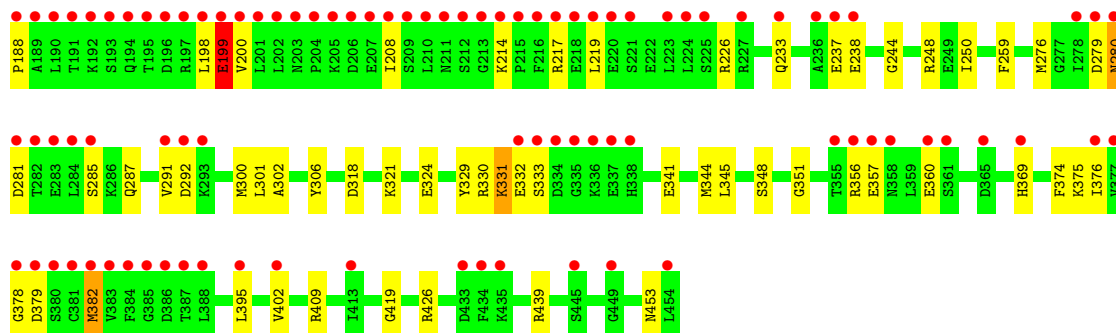
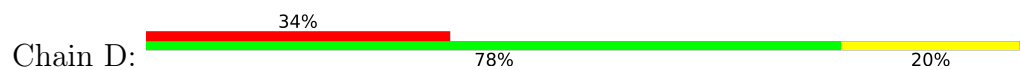


• Molecule 1: Pyrrolysine-tRNA ligase





● Molecule 1: Pyrrolysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.70Å 135.20Å 72.24Å 90.00° 112.54° 90.00°	Depositor
Resolution (Å)	66.72 – 2.15 66.72 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.1 (66.72-2.15) 99.1 (66.72-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.14Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.247 , 0.309 0.247 , 0.307	Depositor DCC
R_{free} test set	3293 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9181	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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: ANP, 2L5

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	0.48	1/2210 (0.0%)	0.76	3/2972 (0.1%)
1	B	0.47	0/2210	0.76	4/2972 (0.1%)
1	C	0.57	2/2210 (0.1%)	0.92	12/2972 (0.4%)
1	D	0.51	2/2210 (0.1%)	0.90	9/2972 (0.3%)
All	All	0.51	5/8840 (0.1%)	0.84	28/11888 (0.2%)

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	1
1	C	0	2
1	D	0	1
All	All	0	4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	375	LYS	CD-CE	12.09	1.88	1.52
1	C	375	LYS	CG-CD	5.96	1.70	1.52
1	D	199	GLU	CD-OE2	5.75	1.36	1.25
1	A	314	ARG	NE-CZ	-5.35	1.27	1.33
1	D	200	VAL	CA-CB	-5.21	1.48	1.54

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	375	LYS	CG-CD-CE	-23.33	57.64	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	GLU	CG-CD-OE1	19.06	162.24	118.40
1	D	199	GLU	CG-CD-OE2	-13.96	86.29	118.40
1	D	199	GLU	OE1-CD-OE2	-12.24	93.52	122.90
1	C	217	ARG	CG-CD-NE	-10.26	89.43	112.00
1	C	375	LYS	CB-CA-C	7.87	126.09	110.42
1	C	375	LYS	CA-C-N	7.18	132.34	122.93
1	C	375	LYS	C-N-CA	7.18	132.34	122.93
1	D	198	LEU	CA-C-N	-6.97	109.40	121.66
1	D	198	LEU	C-N-CA	-6.97	109.40	121.66
1	C	375	LYS	CA-CB-CG	-6.50	101.10	114.10
1	C	229	LYS	CB-CG-CD	6.03	125.18	111.30
1	D	292	ASP	CB-CA-C	-6.02	108.40	117.07
1	B	233	GLN	CB-CA-C	-6.00	101.46	110.88
1	C	217	ARG	CB-CG-CD	5.88	124.82	111.30
1	B	202	LEU	CA-C-N	5.86	136.10	121.80
1	B	202	LEU	C-N-CA	5.86	136.10	121.80
1	D	291	VAL	CA-C-N	-5.53	117.07	123.04
1	D	291	VAL	C-N-CA	-5.53	117.07	123.04
1	A	233	GLN	CA-CB-CG	-5.48	103.14	114.10
1	C	217	ARG	CA-CB-CG	-5.40	103.31	114.10
1	D	199	GLU	CB-CG-CD	5.38	121.74	112.60
1	C	375	LYS	N-CA-CB	-5.35	101.45	110.49
1	C	291	VAL	CA-C-N	5.22	131.51	121.54
1	C	291	VAL	C-N-CA	5.22	131.51	121.54
1	A	286	LYS	CA-C-N	-5.16	114.03	122.54
1	A	286	LYS	C-N-CA	-5.16	114.03	122.54
1	B	382	MET	N-CA-CB	5.02	117.35	109.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	GLU	Sidechain
1	C	292	ASP	Sidechain
1	C	374	PHE	Peptide
1	D	199	GLU	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	2168	0	2175	40	1
1	B	2168	0	2175	71	2
1	C	2168	0	2175	51	1
1	D	2168	0	2175	52	1
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	0
3	A	13	0	4	8	0
3	B	13	0	4	10	0
3	C	13	0	4	3	0
3	D	13	0	4	9	0
4	A	100	0	0	6	0
4	B	89	0	0	10	2
4	C	61	0	0	2	0
4	D	83	0	0	16	2
All	All	9181	0	8768	209	5

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 12.

All (209) 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:D:233:GLN:O	4:D:601:HOH:O	1.80	0.98
1:D:369:HIS:ND1	4:D:602:HOH:O	1.99	0.94
1:B:257:ARG:NH1	4:B:602:HOH:O	1.94	0.92
1:B:348:SER:OG	3:B:502:2L5:CL	2.30	0.86
1:B:349:GLN:OE1	4:B:601:HOH:O	1.94	0.84
1:D:217:ARG:HD2	1:D:217:ARG:N	1.95	0.81
1:A:256:ASP:OD1	4:A:601:HOH:O	1.99	0.81
1:A:302:ALA:HB1	3:A:502:2L5:H4	1.64	0.80
1:B:454:LEU:OXT	4:B:603:HOH:O	1.98	0.80
1:A:394:ASP:OD2	4:A:602:HOH:O	2.00	0.79
1:B:238:GLU:O	4:B:604:HOH:O	1.98	0.79
1:D:238:GLU:C	4:D:604:HOH:O	2.24	0.79
1:D:238:GLU:O	4:D:604:HOH:O	2.02	0.78
1:C:287:GLN:NE2	1:C:332:GLU:HB3	2.00	0.77
1:D:331:LYS:O	4:D:605:HOH:O	2.03	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:SER:OG	3:A:502:2L5:CL	2.41	0.75
1:A:379:ASP:HB3	1:A:382:MET:HB2	1.67	0.75
1:C:302:ALA:HB1	3:C:502:2L5:H4	1.70	0.74
1:D:302:ALA:HB1	3:D:502:2L5:H4	1.70	0.74
1:C:419:GLY:HA3	3:C:502:2L5:CL	2.24	0.73
1:C:333:SER:HB2	1:C:340:GLU:HG3	1.69	0.72
1:A:306:TYR:CG	3:A:502:2L5:H3	2.25	0.72
1:B:356:ARG:HH12	1:B:379:ASP:CB	2.03	0.71
1:B:356:ARG:NH2	1:B:379:ASP:O	2.17	0.70
3:D:502:2L5:N	4:D:607:HOH:O	2.25	0.70
1:B:214:LYS:HE2	1:B:219:LEU:HD21	1.74	0.69
1:C:228:LYS:NZ	4:C:601:HOH:O	2.12	0.69
1:D:356:ARG:HB3	1:D:402:VAL:HG21	1.76	0.68
1:A:282:THR:HG22	1:A:283:GLU:H	1.57	0.68
1:B:287:GLN:HA	1:B:331:LYS:HB2	1.75	0.68
1:A:299:PRO:HG2	1:A:300:MET:HE2	1.76	0.67
1:B:359:LEU:HD21	1:B:400:ALA:HB1	1.79	0.65
1:C:379:ASP:HB3	1:C:382:MET:HB2	1.77	0.65
1:C:225:SER:O	1:C:229:LYS:HG2	1.97	0.64
1:C:240:GLU:OE1	4:C:602:HOH:O	2.15	0.64
1:A:377:VAL:HG22	1:A:389:ASP:HB2	1.80	0.64
1:D:333:SER:N	4:D:605:HOH:O	2.30	0.64
1:C:284:LEU:HD21	1:C:300:MET:HE1	1.79	0.63
1:A:278:ILE:HD11	1:A:284:LEU:HD23	1.79	0.63
1:A:287:GLN:OE1	1:A:332:GLU:HB3	1.99	0.63
1:B:415:LYS:NZ	4:B:605:HOH:O	2.09	0.62
1:A:212:SER:OG	1:A:213:GLY:N	2.33	0.62
1:D:348:SER:OG	3:D:502:2L5:H1	1.99	0.62
1:C:287:GLN:HE21	1:C:332:GLU:HB3	1.62	0.62
1:B:360:GLU:HG2	1:B:376:ILE:HD13	1.82	0.61
1:D:378:GLY:HA2	4:D:669:HOH:O	2.01	0.61
1:B:212:SER:HB2	1:B:214:LYS:NZ	2.15	0.61
1:B:379:ASP:OD2	1:B:382:MET:HB3	2.02	0.60
1:D:409:ARG:NH1	4:D:610:HOH:O	2.26	0.60
1:A:306:TYR:CD2	3:A:502:2L5:H3	2.36	0.60
1:B:387:THR:HG22	1:B:401:VAL:HG22	1.82	0.60
1:D:208:ILE:HB	1:D:226:ARG:HH22	1.67	0.60
1:B:275:ARG:NH2	4:B:610:HOH:O	2.30	0.60
1:B:302:ALA:HB1	3:B:502:2L5:H4	1.83	0.59
1:B:356:ARG:HH11	1:B:382:MET:HG2	1.67	0.59
1:D:287:GLN:HE21	1:D:330:ARG:HB3	1.65	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:MET:HA	1:D:344:MET:HE1	1.86	0.58
1:D:279:ASP:O	1:D:281:ASP:N	2.30	0.58
1:D:419:GLY:HA3	3:D:502:2L5:CL	2.41	0.58
1:B:189:ALA:H	1:C:281:ASP:CG	2.12	0.57
1:A:279:ASP:C	1:A:281:ASP:H	2.13	0.56
1:C:195:THR:O	1:C:199:GLU:HG2	2.06	0.56
1:D:199:GLU:O	1:D:439:ARG:NH2	2.38	0.56
1:C:215:PRO:C	1:C:217:ARG:H	2.15	0.55
1:C:194:GLN:HG2	1:C:216:PHE:CD2	2.42	0.55
1:D:374:PHE:C	1:D:375:LYS:HD3	2.32	0.54
1:A:359:LEU:HD21	1:A:400:ALA:HB1	1.89	0.54
1:D:279:ASP:C	1:D:281:ASP:H	2.15	0.54
1:A:226:ARG:NH1	4:A:604:HOH:O	2.20	0.54
1:B:212:SER:HB2	1:B:214:LYS:HZ2	1.72	0.54
1:B:321:LYS:HG2	1:B:349:GLN:HG3	1.89	0.54
1:B:414:ASP:N	1:B:414:ASP:OD1	2.36	0.54
1:D:279:ASP:O	1:D:285:SER:OG	2.17	0.54
1:D:188:PRO:N	4:D:615:HOH:O	2.41	0.53
1:B:356:ARG:HH12	1:B:379:ASP:HB3	1.73	0.53
1:D:356:ARG:NE	1:D:382:MET:HE1	2.25	0.52
1:B:192:LYS:HG2	1:C:270:LEU:CD2	2.39	0.52
1:C:302:ALA:CB	3:C:502:2L5:H4	2.39	0.52
1:C:287:GLN:HA	1:C:331:LYS:HB2	1.90	0.52
1:B:356:ARG:HH22	1:B:379:ASP:C	2.10	0.52
1:A:302:ALA:CB	3:A:502:2L5:H4	2.39	0.51
1:B:415:LYS:CE	4:B:605:HOH:O	2.55	0.51
1:A:192:LYS:HA	1:A:195:THR:HG22	1.91	0.51
1:A:235:TYR:CG	1:C:316:LEU:HD13	2.45	0.51
1:B:214:LYS:CE	1:B:219:LEU:HD21	2.40	0.51
1:D:329:TYR:CE2	1:D:341:GLU:HG3	2.45	0.51
1:D:306:TYR:CG	3:D:502:2L5:H3	2.46	0.51
1:B:266:ILE:HA	1:B:298:ARG:HD3	1.92	0.50
1:A:372:ILE:O	4:A:603:HOH:O	2.19	0.50
1:A:309:LEU:HD12	3:A:502:2L5:H2	1.93	0.50
1:D:287:GLN:HA	1:D:331:LYS:HB2	1.94	0.50
1:C:215:PRO:C	1:C:217:ARG:N	2.68	0.49
1:D:301:LEU:HD13	1:D:324:GLU:HB3	1.95	0.49
1:C:275:ARG:O	1:C:407:LEU:HD11	2.12	0.49
1:C:300:MET:HA	1:C:344:MET:HE1	1.94	0.49
1:D:360:GLU:OE1	1:D:376:ILE:HD12	2.13	0.49
1:A:333:SER:CB	1:A:340:GLU:HG3	2.43	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:GLU:HB2	4:D:601:HOH:O	2.13	0.49
1:D:453:ASN:ND2	4:D:612:HOH:O	2.30	0.49
1:D:306:TYR:CD2	3:D:502:2L5:H3	2.48	0.49
1:D:318:ASP:OD1	1:D:351:GLY:HA3	2.13	0.48
1:D:348:SER:OG	3:D:502:2L5:C19	2.61	0.48
1:D:382:MET:HE3	1:D:382:MET:HB3	1.79	0.48
1:B:318:ASP:OD2	1:B:352:SER:OG	2.28	0.48
1:B:306:TYR:CE2	3:B:502:2L5:H3	2.49	0.48
1:B:346:ASP:OD1	3:B:502:2L5:CL	2.69	0.48
1:B:244:GLY:O	1:B:248:ARG:HG3	2.14	0.48
1:D:214:LYS:HE2	1:D:219:LEU:CD2	2.44	0.48
1:B:189:ALA:N	1:C:281:ASP:OD1	2.45	0.47
1:B:337:GLU:OE2	1:B:429:LYS:HE3	2.14	0.47
1:B:356:ARG:HB2	1:B:402:VAL:HG21	1.97	0.47
1:C:191:THR:HG23	1:C:194:GLN:H	1.79	0.47
1:C:360:GLU:HG2	1:C:376:ILE:HD13	1.97	0.47
1:C:414:ASP:O	1:C:414:ASP:OD1	2.32	0.47
1:D:244:GLY:O	1:D:248:ARG:HG3	2.14	0.47
1:B:278:ILE:HG22	1:B:285:SER:HB2	1.96	0.47
1:D:379:ASP:OD2	1:D:382:MET:HB2	2.14	0.47
1:B:199:GLU:O	1:B:435:LYS:NZ	2.48	0.46
1:B:300:MET:HG2	1:B:302:ALA:H	1.80	0.46
1:B:360:GLU:HG2	1:B:376:ILE:CD1	2.46	0.46
1:A:394:ASP:CG	4:A:602:HOH:O	2.55	0.46
1:B:306:TYR:CD2	3:B:502:2L5:H3	2.51	0.46
1:A:246:LEU:O	1:A:250:ILE:HG13	2.16	0.46
1:D:208:ILE:HB	1:D:226:ARG:NH2	2.31	0.46
1:C:266:ILE:HA	1:C:298:ARG:HD3	1.98	0.46
1:C:318:ASP:OD1	1:C:351:GLY:HA3	2.16	0.45
1:B:379:ASP:HB2	1:B:382:MET:HE2	1.97	0.45
1:C:359:LEU:HB2	1:C:418:ILE:HD12	1.98	0.45
1:D:250:ILE:HG21	1:D:345:LEU:HD22	1.98	0.45
1:C:253:PHE:O	1:C:257:ARG:HD3	2.16	0.45
1:A:333:SER:HB3	1:A:340:GLU:HG3	1.99	0.45
1:A:228:LYS:HE2	1:C:314:ARG:O	2.17	0.45
1:A:282:THR:HG22	1:A:283:GLU:N	2.29	0.45
1:C:191:THR:HG22	1:C:194:GLN:CD	2.42	0.45
1:D:276:MET:HG3	1:D:300:MET:HE1	1.99	0.45
1:A:303:PRO:HB3	1:A:411:TRP:CH2	2.52	0.45
1:B:294:ASN:N	4:B:616:HOH:O	2.39	0.45
1:B:436:ASN:HD21	1:B:438:LYS:NZ	2.14	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ASN:HB3	1:C:204:PRO:CD	2.47	0.45
1:C:244:GLY:O	1:C:248:ARG:HG3	2.16	0.45
1:C:414:ASP:O	1:C:415:LYS:HG3	2.17	0.45
1:C:227:ARG:HD3	1:C:450:ILE:HG23	1.98	0.45
1:C:194:GLN:HG2	1:C:216:PHE:CG	2.52	0.44
1:C:284:LEU:HD21	1:C:300:MET:CE	2.45	0.44
1:C:356:ARG:HB3	1:C:402:VAL:HG21	1.99	0.44
1:A:382:MET:HG3	1:A:386:ASP:CB	2.47	0.44
1:B:306:TYR:CZ	3:B:502:2L5:H3	2.52	0.44
1:B:356:ARG:HH12	1:B:379:ASP:HB2	1.80	0.44
1:A:327:PRO:HA	1:A:342:PHE:O	2.17	0.44
1:B:345:LEU:O	1:B:421:GLY:HA2	2.17	0.44
1:C:259:PHE:CD2	1:C:321:LYS:HB3	2.53	0.44
1:A:208:ILE:N	4:A:604:HOH:O	2.51	0.44
1:A:382:MET:HG3	1:A:386:ASP:HB2	2.00	0.44
1:B:404:PRO:HB3	4:B:612:HOH:O	2.17	0.44
1:B:380:SER:HB2	1:B:381:CYS:H	1.58	0.44
1:B:436:ASN:OD1	1:B:438:LYS:HG3	2.17	0.44
1:C:203:ASN:OD1	1:C:227:ARG:CZ	2.65	0.44
1:D:348:SER:OG	3:D:502:2L5:CL	2.71	0.44
1:B:270:LEU:HD12	1:B:296:CYS:HB3	1.99	0.44
1:D:332:GLU:C	4:D:605:HOH:O	2.60	0.44
1:B:279:ASP:C	1:B:281:ASP:H	2.25	0.43
1:D:300:MET:HA	1:D:344:MET:CE	2.48	0.43
1:D:395:LEU:HD11	1:D:426:ARG:HD3	2.00	0.43
1:D:331:LYS:C	4:D:605:HOH:O	2.58	0.43
1:B:306:TYR:CD1	3:B:502:2L5:H3	2.53	0.43
1:B:303:PRO:HB3	1:B:411:TRP:CH2	2.54	0.43
1:C:203:ASN:HB3	1:C:204:PRO:HD2	2.01	0.43
1:B:347:PHE:CE2	1:B:420:ALA:HB3	2.54	0.43
1:D:237:GLU:N	4:D:601:HOH:O	2.45	0.43
1:B:379:ASP:OD2	1:B:382:MET:HE2	2.18	0.43
1:B:348:SER:OG	3:B:502:2L5:H1	2.19	0.43
1:C:191:THR:OG1	1:C:192:LYS:N	2.52	0.43
1:C:282:THR:HG22	1:C:283:GLU:H	1.83	0.43
1:B:215:PRO:HD2	1:B:218:GLU:OE1	2.19	0.42
1:B:379:ASP:HB2	1:B:382:MET:CE	2.49	0.42
1:D:259:PHE:CD2	1:D:321:LYS:HB3	2.55	0.42
1:B:302:ALA:HB1	3:B:502:2L5:C16	2.49	0.42
1:A:233:GLN:O	1:A:233:GLN:HG2	2.20	0.42
1:B:222:GLU:O	1:B:225:SER:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:GLN:NE2	1:D:330:ARG:HB3	2.33	0.42
1:B:202:LEU:HG	1:B:203:ASN:H	1.85	0.42
1:B:205:LYS:HE2	1:B:227:ARG:NH2	2.35	0.42
1:B:424:LEU:HA	1:B:427:LEU:HD12	2.02	0.42
1:B:192:LYS:HG2	1:C:270:LEU:HD23	2.02	0.41
1:C:262:ILE:O	1:C:324:GLU:HG3	2.19	0.41
1:D:280:ASN:HA	1:D:285:SER:HB3	2.02	0.41
1:A:306:TYR:CD1	3:A:502:2L5:H3	2.54	0.41
1:A:377:VAL:CG2	1:A:389:ASP:HB2	2.47	0.41
1:B:306:TYR:CE1	3:B:502:2L5:H3	2.55	0.41
1:C:376:ILE:HA	1:C:389:ASP:O	2.21	0.41
1:D:382:MET:C	1:D:382:MET:SD	3.03	0.41
1:B:377:VAL:CG2	1:B:389:ASP:HB2	2.50	0.41
1:A:382:MET:HE3	1:A:382:MET:HB3	1.94	0.41
1:A:284:LEU:HA	1:A:287:GLN:HG3	2.03	0.41
1:B:294:ASN:HB2	4:B:616:HOH:O	2.21	0.41
1:B:282:THR:HG22	1:B:283:GLU:N	2.36	0.41
1:C:357:GLU:CD	1:C:357:GLU:H	2.29	0.41
1:D:238:GLU:CA	4:D:604:HOH:O	2.67	0.41
1:D:302:ALA:CB	3:D:502:2L5:H4	2.47	0.41
1:A:325:ILE:HA	1:A:344:MET:O	2.21	0.41
1:C:280:ASN:HA	1:C:285:SER:OG	2.20	0.41
1:A:348:SER:OG	3:A:502:2L5:H1	2.20	0.40
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.78	0.40
1:B:356:ARG:NH1	1:B:379:ASP:HB2	2.36	0.40
1:A:288:ILE:CD1	1:A:299:PRO:HG3	2.51	0.40
1:C:282:THR:HG22	1:C:283:GLU:N	2.36	0.40
1:B:250:ILE:HG21	1:B:345:LEU:HD22	2.02	0.40
1:C:301:LEU:HD12	1:C:346:ASP:HB2	2.03	0.40
1:C:387:THR:HG22	1:C:401:VAL:HG22	2.03	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:627:HOH:O	4:D:651:HOH:O[1_656]	1.81	0.39
1:B:380:SER:OG	1:D:357:GLU:O[1_556]	1.87	0.33
4:B:614:HOH:O	4:D:622:HOH:O[1_656]	2.03	0.17
1:A:238:GLU:OE2	1:B:245:LYS:NZ[2_646]	2.16	0.04
1:C:217:ARG:NH2	1:C:414:ASP:O[1_455]	2.16	0.04

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	265/267 (99%)	249 (94%)	13 (5%)	3 (1%)	11	7
1	B	265/267 (99%)	241 (91%)	24 (9%)	0	100	100
1	C	265/267 (99%)	249 (94%)	14 (5%)	2 (1%)	16	10
1	D	265/267 (99%)	246 (93%)	16 (6%)	3 (1%)	11	7
All	All	1060/1068 (99%)	985 (93%)	67 (6%)	8 (1%)	16	10

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	375	LYS
1	D	382	MET
1	A	314	ARG
1	D	280	ASN
1	C	216	PHE
1	A	212	SER
1	A	280	ASN
1	D	331	LYS

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	241/241 (100%)	241 (100%)	0	100	100
1	B	241/241 (100%)	240 (100%)	1 (0%)	84	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	241/241 (100%)	240 (100%)	1 (0%)	84	89
1	D	241/241 (100%)	241 (100%)	0	100	100
All	All	964/964 (100%)	962 (100%)	2 (0%)	87	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	SER
1	C	375	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	304	ASN
1	A	338	HIS
1	B	203	ASN
1	B	287	GLN
1	C	194	GLN
1	C	233	GLN
1	C	294	ASN
1	C	338	HIS
1	C	368	ASN
1	D	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	2L5	D	502	-	12,13,13	1.19	1 (8%)	11,17,17	1.21	1 (9%)
2	ANP	A	501	-	33,33,33	1.11	5 (15%)	45,52,52	0.74	2 (4%)
3	2L5	A	502	-	12,13,13	1.04	1 (8%)	11,17,17	1.38	3 (27%)
3	2L5	C	502	-	12,13,13	1.14	1 (8%)	11,17,17	1.04	0
3	2L5	B	502	-	12,13,13	1.03	1 (8%)	11,17,17	0.83	0
2	ANP	B	501	-	33,33,33	1.09	5 (15%)	45,52,52	0.75	1 (2%)
2	ANP	D	501	-	33,33,33	1.09	4 (12%)	45,52,52	0.75	2 (4%)
2	ANP	C	501	-	33,33,33	1.11	4 (12%)	45,52,52	0.74	2 (4%)

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	2L5	D	502	-	-	4/8/8/8	0/1/1/1
2	ANP	A	501	-	-	7/18/38/38	0/3/3/3
3	2L5	A	502	-	-	1/8/8/8	0/1/1/1
3	2L5	C	502	-	-	4/8/8/8	0/1/1/1
3	2L5	B	502	-	-	1/8/8/8	0/1/1/1
2	ANP	B	501	-	-	4/18/38/38	0/3/3/3
2	ANP	D	501	-	-	7/18/38/38	0/3/3/3
2	ANP	C	501	-	-	8/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ANP	PG-O1G	3.26	1.51	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	ANP	PB-O1B	3.12	1.50	1.46
3	D	502	2L5	C15-CL	3.04	1.80	1.73
2	A	501	ANP	PG-O1G	3.02	1.50	1.46
2	D	501	ANP	PG-N3B	3.01	1.71	1.63
2	B	501	ANP	PG-O1G	3.01	1.50	1.46
2	B	501	ANP	PB-O1B	2.97	1.50	1.46
2	A	501	ANP	PG-N3B	2.97	1.71	1.63
2	D	501	ANP	PG-O1G	2.93	1.50	1.46
3	C	502	2L5	C15-CL	2.92	1.80	1.73
2	D	501	ANP	PB-O1B	2.90	1.50	1.46
2	C	501	ANP	PG-N3B	2.90	1.70	1.63
2	B	501	ANP	PG-N3B	2.81	1.70	1.63
2	C	501	ANP	PB-O1B	2.77	1.50	1.46
2	B	501	ANP	PB-O3A	-2.56	1.55	1.59
2	D	501	ANP	PB-N3B	2.47	1.69	1.63
3	A	502	2L5	C15-CL	2.39	1.79	1.73
2	C	501	ANP	PB-N3B	2.34	1.69	1.63
3	B	502	2L5	C15-CL	2.17	1.78	1.73
2	A	501	ANP	PB-O3A	-2.14	1.56	1.59
2	A	501	ANP	PB-N3B	2.14	1.69	1.63
2	B	501	ANP	PB-N3B	2.10	1.68	1.63

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	ANP	O1G-PG-N3B	-2.83	107.60	111.77
2	D	501	ANP	O1B-PB-N3B	-2.60	107.95	111.77
2	C	501	ANP	O3G-PG-O1G	-2.53	107.12	113.45
3	D	502	2L5	C17-C18-C19	-2.50	117.16	120.24
2	C	501	ANP	O1B-PB-N3B	-2.47	108.14	111.77
3	A	502	2L5	C14-C15-CL	-2.43	115.89	119.75
2	A	501	ANP	O2G-PG-O1G	-2.20	107.93	113.45
3	A	502	2L5	C19-C15-CL	2.08	122.52	118.42
2	D	501	ANP	O2G-PG-O1G	-2.05	108.31	113.45
3	A	502	2L5	C17-C18-C19	-2.05	117.71	120.24
2	A	501	ANP	O3G-PG-O1G	-2.02	108.39	113.45

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ANP	PB-N3B-PG-O1G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	501	ANP	PG-N3B-PB-O1B
2	A	501	ANP	PA-O3A-PB-O1B
2	A	501	ANP	C5'-O5'-PA-O2A
2	A	501	ANP	C5'-O5'-PA-O3A
2	B	501	ANP	PB-N3B-PG-O1G
2	B	501	ANP	PG-N3B-PB-O1B
2	C	501	ANP	PB-N3B-PG-O1G
2	C	501	ANP	C5'-O5'-PA-O2A
2	D	501	ANP	PB-N3B-PG-O1G
2	D	501	ANP	PG-N3B-PB-O1B
2	D	501	ANP	PA-O3A-PB-O2B
2	D	501	ANP	C5'-O5'-PA-O1A
2	D	501	ANP	C5'-O5'-PA-O2A
2	D	501	ANP	C5'-O5'-PA-O3A
3	C	502	2L5	C14-C13-CA-C
3	D	502	2L5	C14-C13-CA-C
3	D	502	2L5	C14-C13-CA-N
3	D	502	2L5	OXT-C-CA-C13
2	C	501	ANP	PG-N3B-PB-O3A
2	A	501	ANP	C5'-O5'-PA-O1A
2	C	501	ANP	C5'-O5'-PA-O1A
2	C	501	ANP	C5'-O5'-PA-O3A
3	B	502	2L5	C14-C13-CA-C
3	C	502	2L5	C14-C13-CA-N
3	D	502	2L5	O-C-CA-C13
3	C	502	2L5	O-C-CA-C13
3	C	502	2L5	OXT-C-CA-C13
2	C	501	ANP	PG-N3B-PB-O1B
2	B	501	ANP	C4'-C5'-O5'-PA
2	A	501	ANP	C4'-C5'-O5'-PA
3	A	502	2L5	C14-C13-CA-C
2	C	501	ANP	C4'-C5'-O5'-PA
2	B	501	ANP	PA-O3A-PB-O1B
2	C	501	ANP	PA-O3A-PB-O1B
2	D	501	ANP	PA-O3A-PB-O1B

There are no ring outliers.

4 monomers are involved in 30 short contacts:

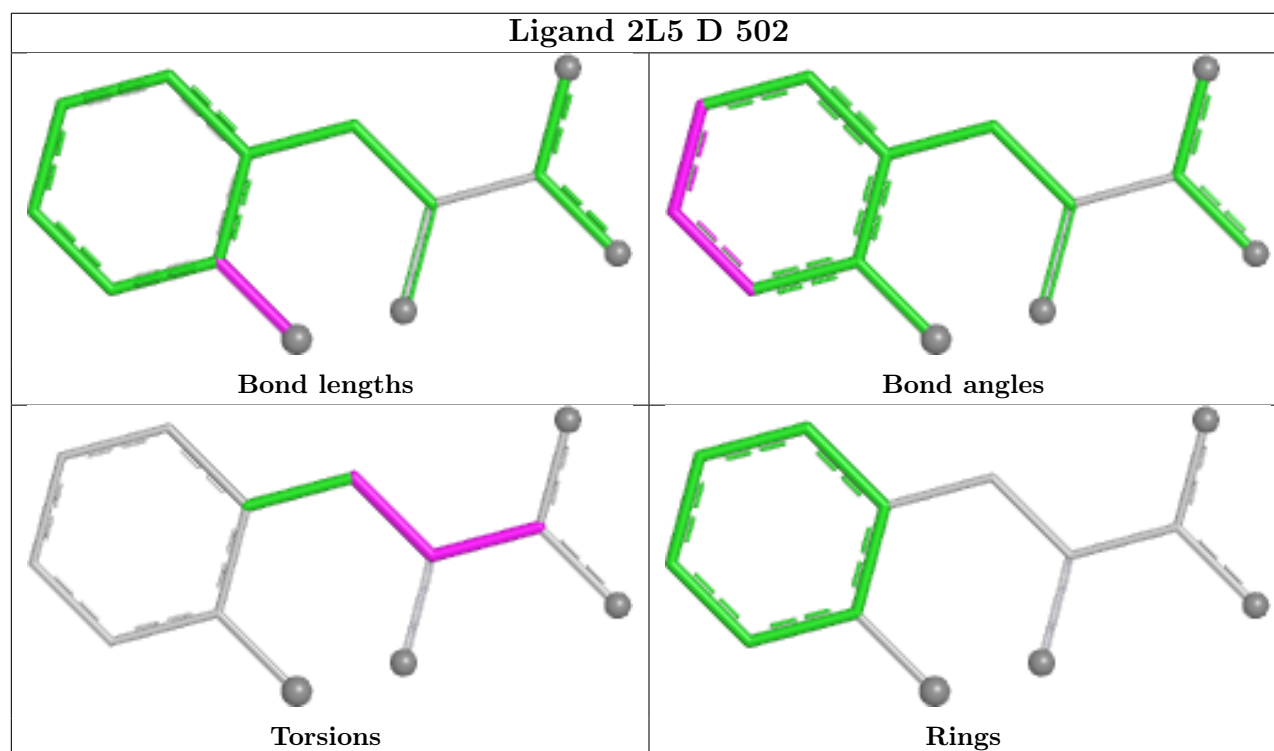
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	502	2L5	9	0
3	A	502	2L5	8	0

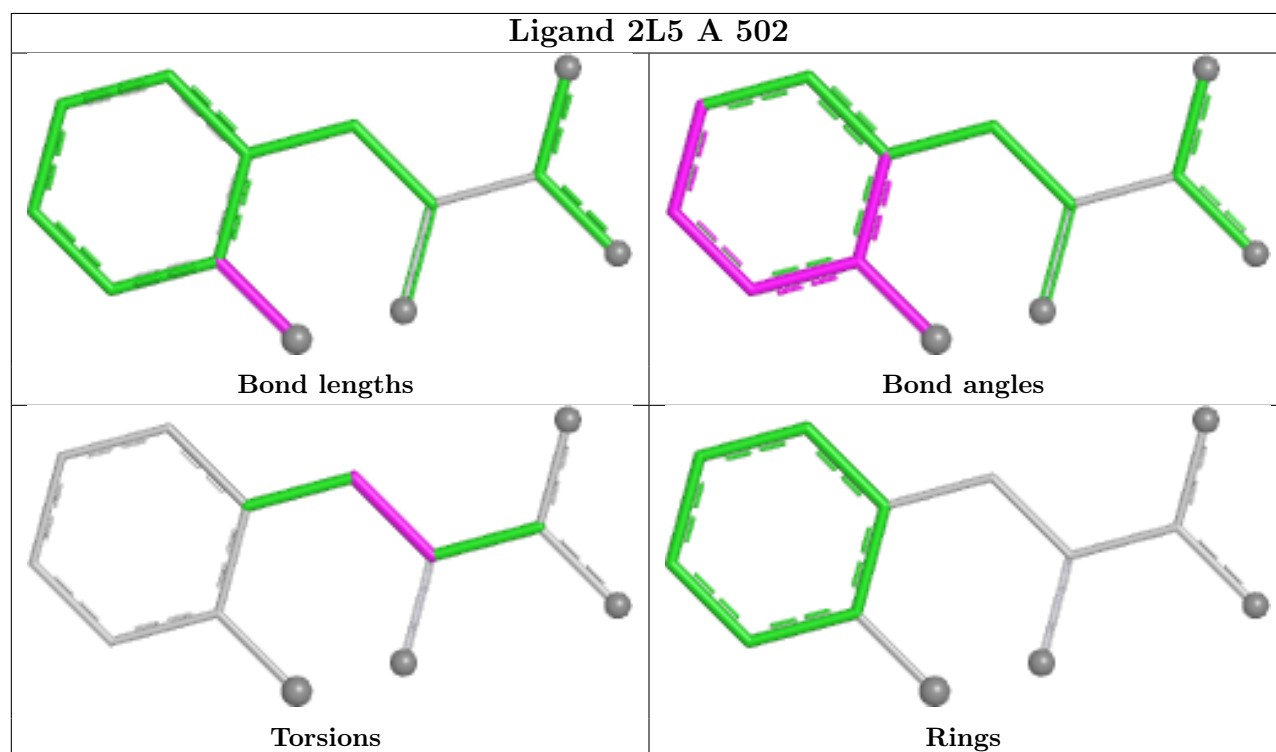
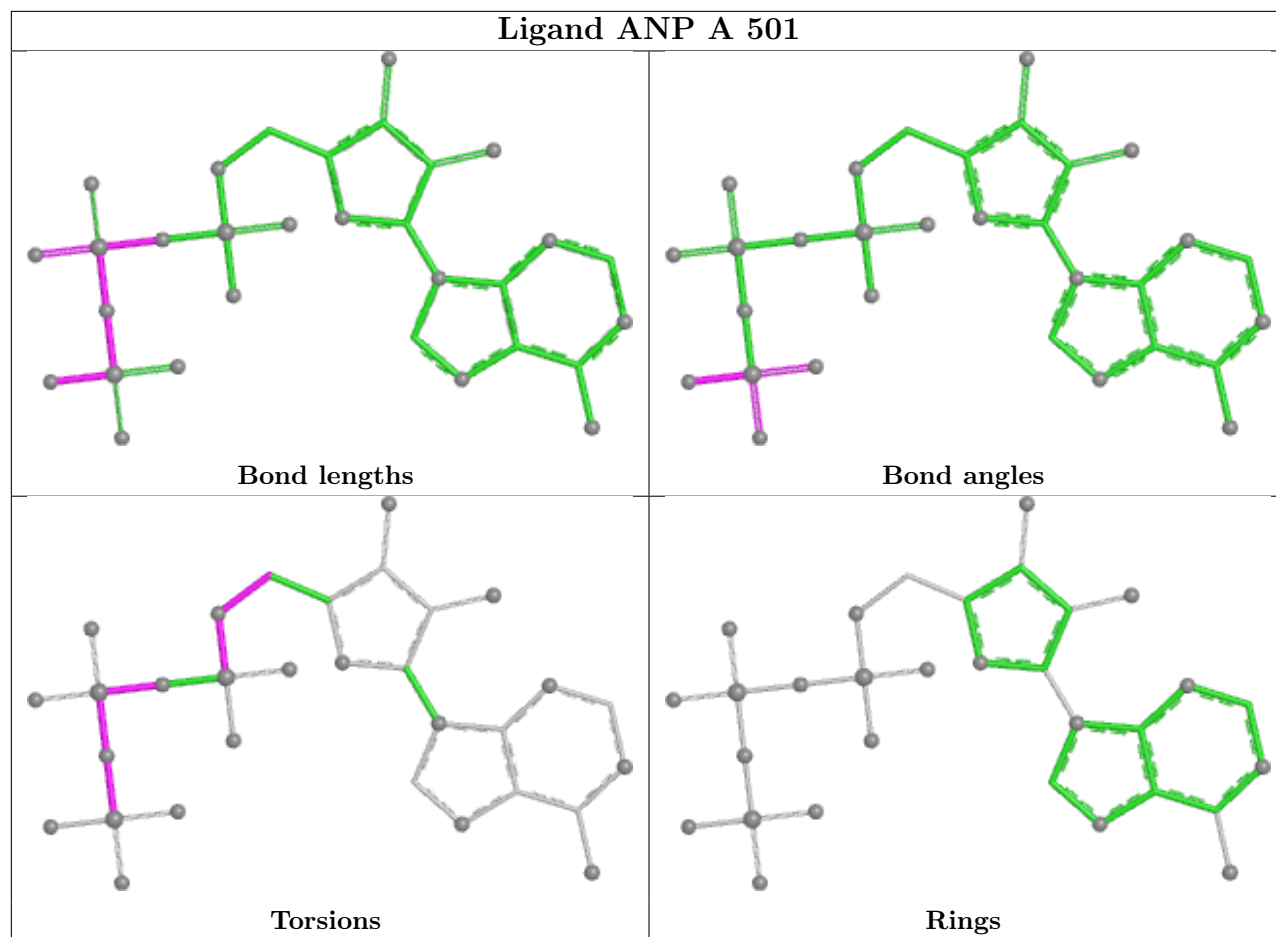
Continued on next page...

Continued from previous page...

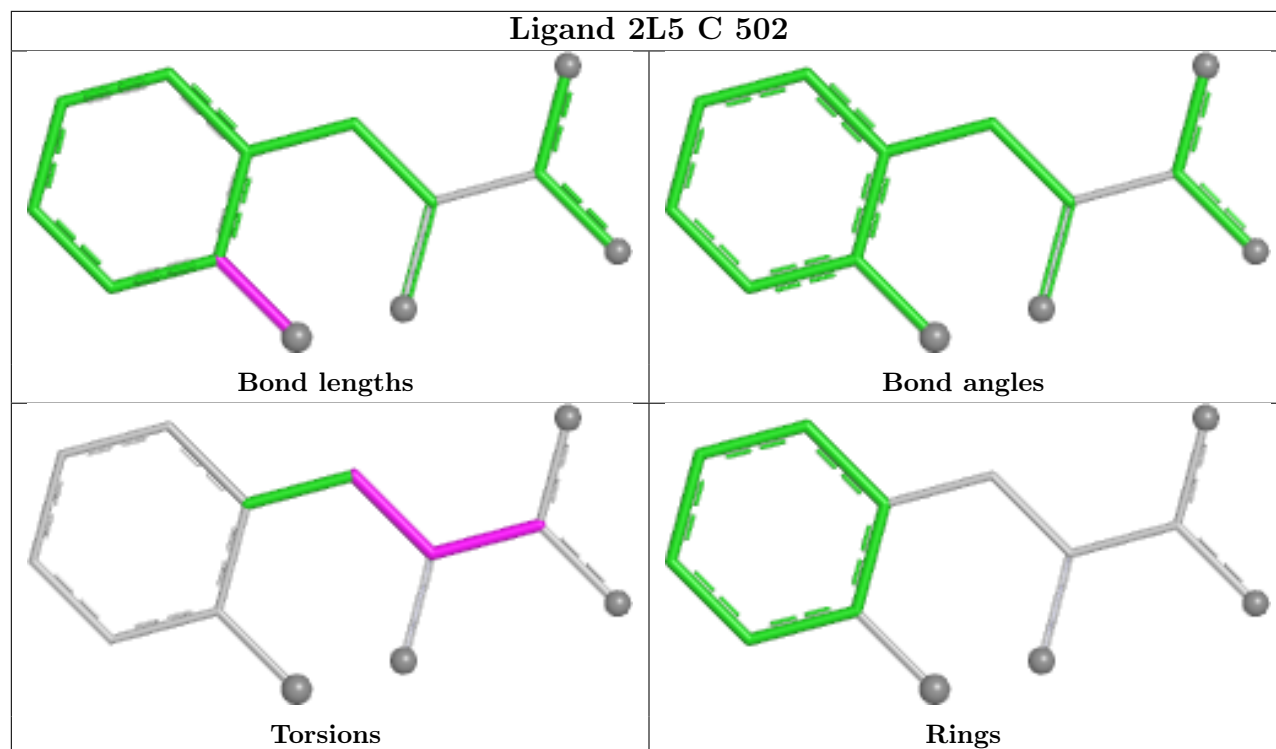
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	502	2L5	3	0
3	B	502	2L5	10	0

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.

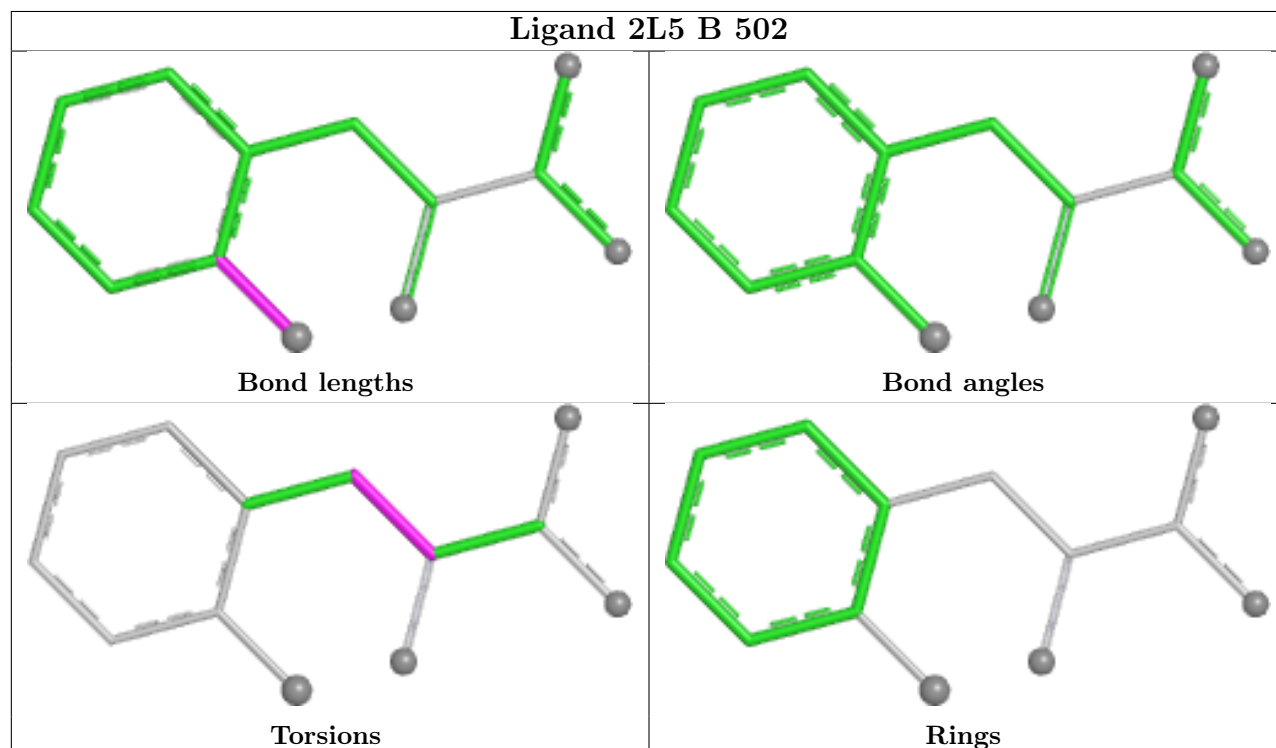


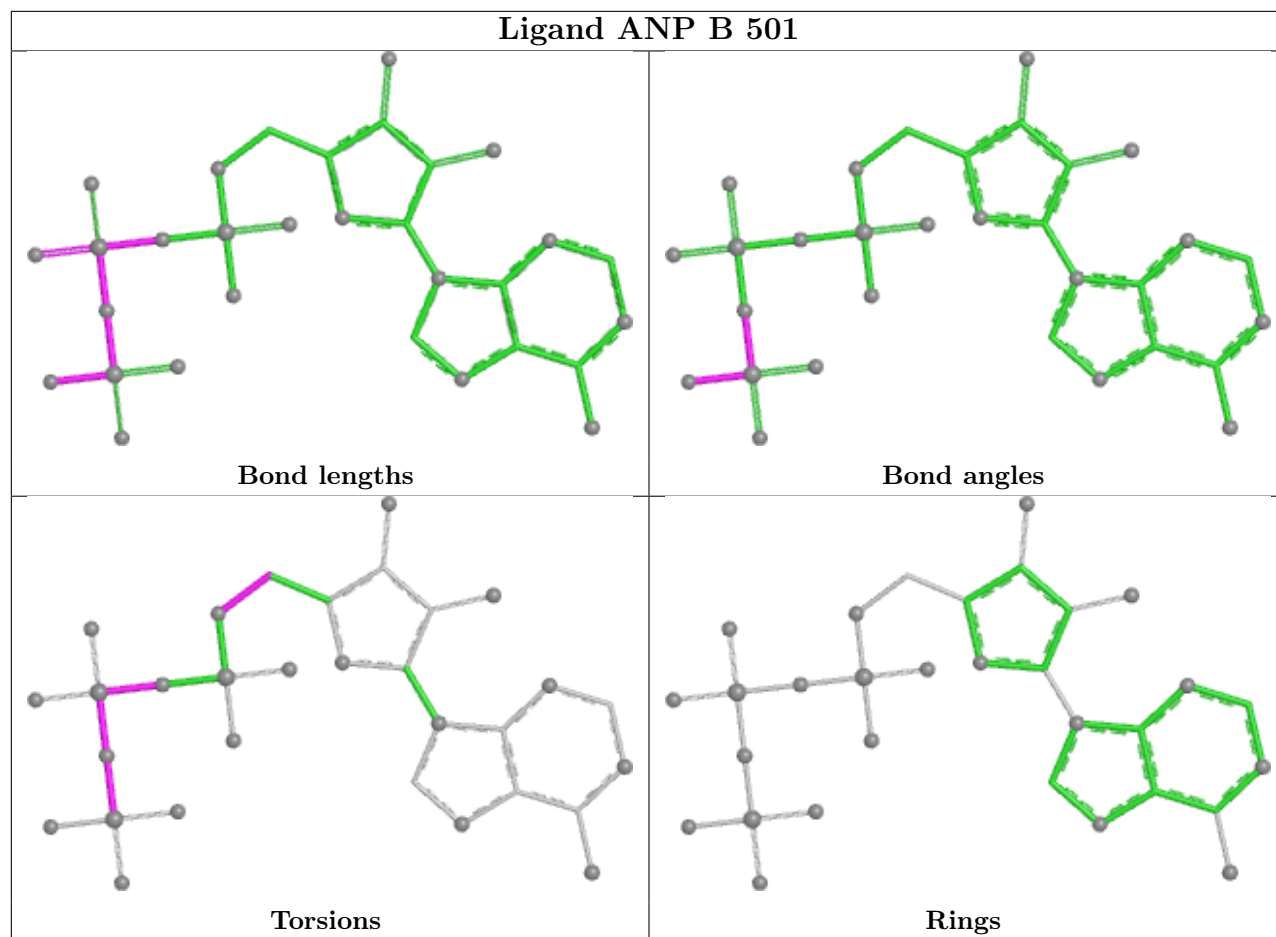


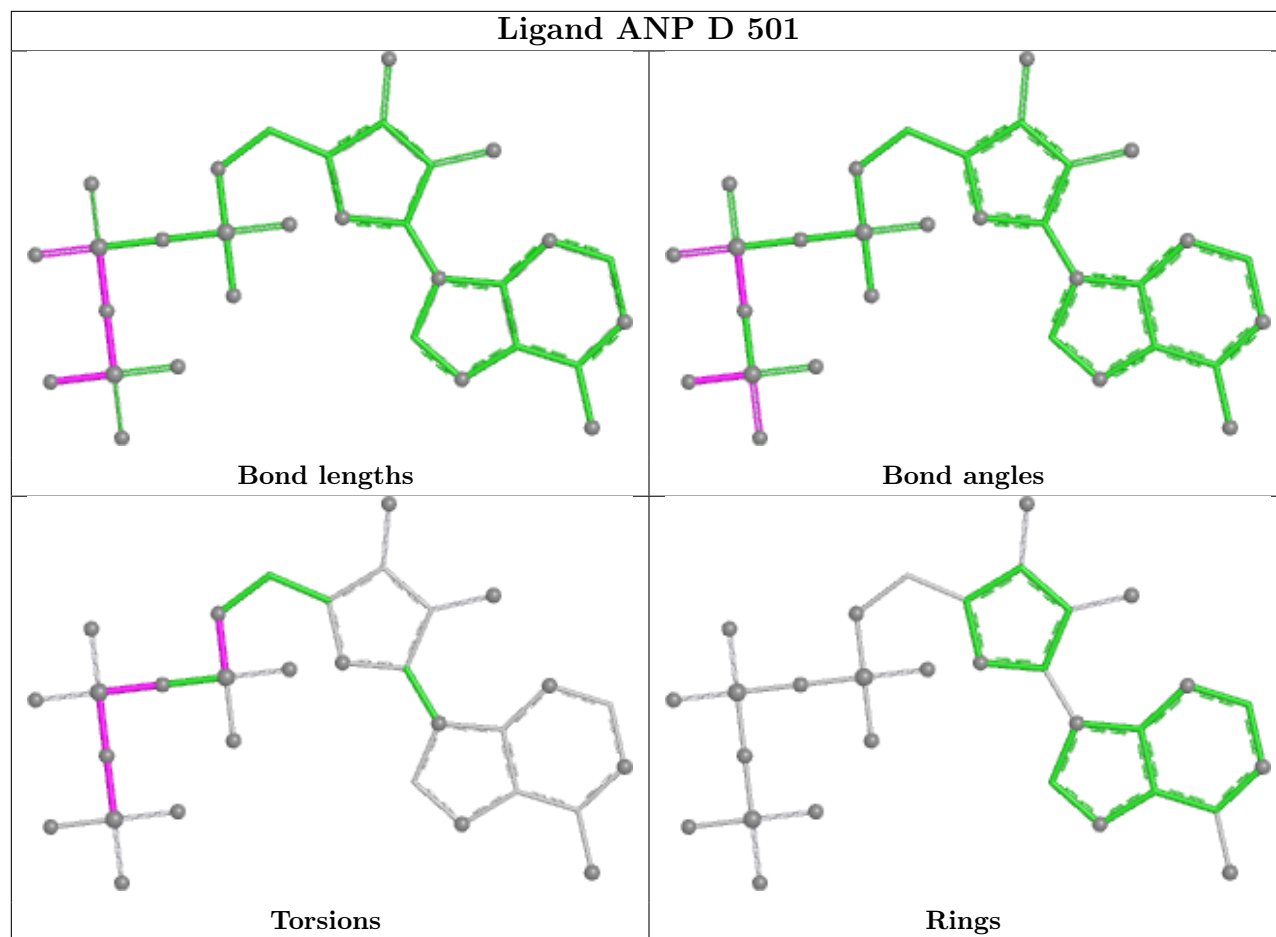
Ligand 2L5 C 502

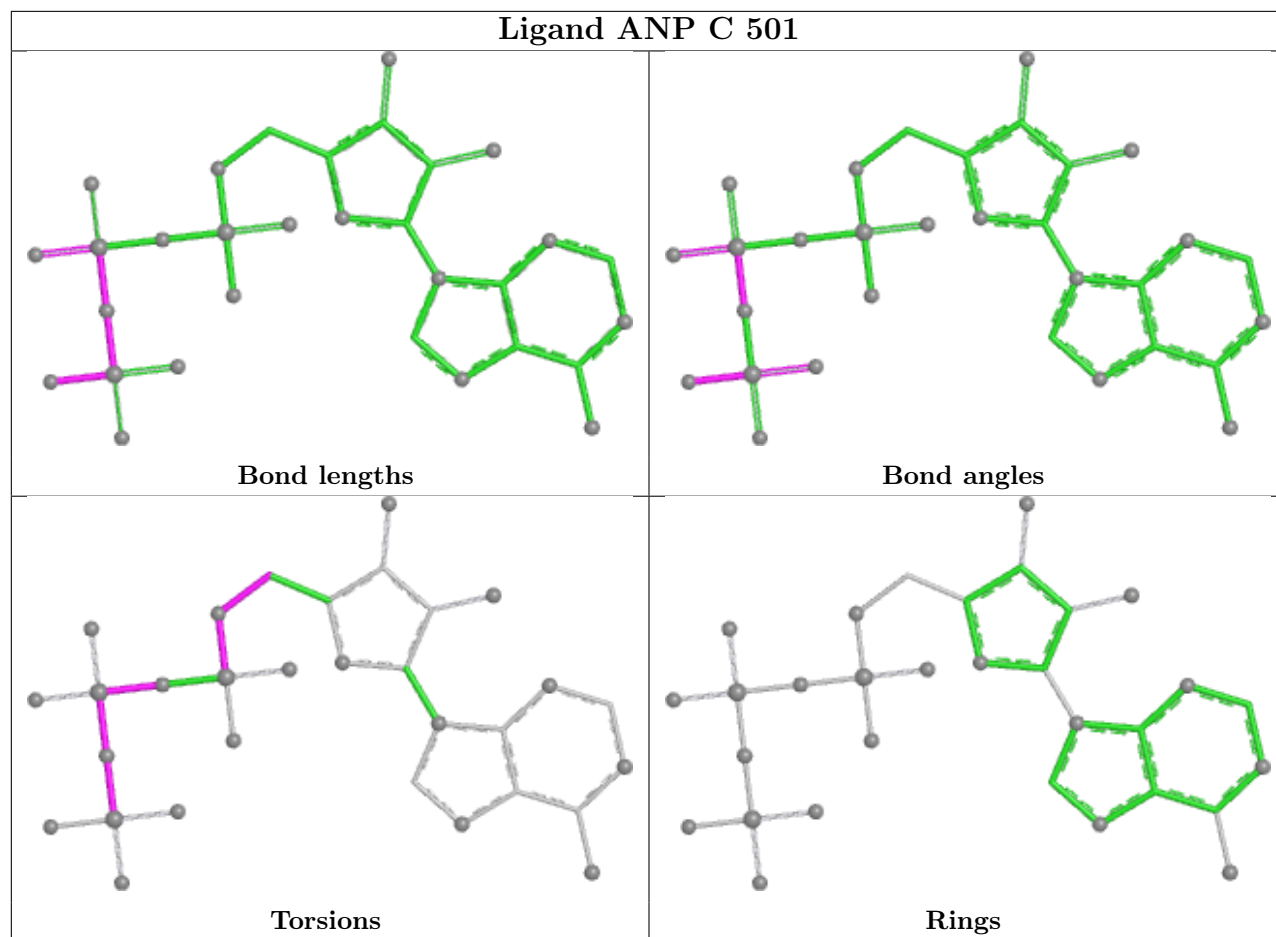


Ligand 2L5 B 502









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/267 (100%)	1.20	51 (19%) 3 4	22, 35, 77, 99	0
1	B	267/267 (100%)	1.48	62 (23%) 2 2	21, 38, 83, 97	0
1	C	267/267 (100%)	1.52	75 (28%) 1 1	22, 39, 86, 103	0
1	D	267/267 (100%)	1.74	90 (33%) 1 1	22, 39, 86, 99	0
All	All	1068/1068 (100%)	1.49	278 (26%) 1 2	21, 38, 82, 103	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	SER	9.5
1	C	279	ASP	8.6
1	B	379	ASP	8.1
1	B	378	GLY	8.0
1	B	383	VAL	7.8
1	C	210	LEU	7.2
1	D	383	VAL	7.2
1	B	384	PHE	7.1
1	D	279	ASP	7.1
1	D	382	MET	6.9
1	B	208	ILE	6.7
1	B	189	ALA	6.6
1	C	208	ILE	6.3
1	D	334	ASP	6.2
1	C	282	THR	6.1
1	D	384	PHE	6.1
1	A	282	THR	6.1
1	D	208	ILE	5.9
1	D	380	SER	5.9
1	D	282	THR	5.9
1	C	381	CYS	5.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	212	SER	5.7
1	D	278	ILE	5.7
1	B	188	PRO	5.7
1	B	282	THR	5.6
1	C	334	ASP	5.6
1	C	335	GLY	5.6
1	B	381	CYS	5.6
1	D	385	GLY	5.6
1	A	189	ALA	5.5
1	C	204	PRO	5.5
1	D	381	CYS	5.4
1	D	210	LEU	5.3
1	B	382	MET	5.3
1	C	213	GLY	5.3
1	D	204	PRO	5.2
1	B	204	PRO	5.2
1	D	379	ASP	5.1
1	A	383	VAL	5.0
1	A	204	PRO	5.0
1	B	211	ASN	5.0
1	A	210	LEU	5.0
1	C	383	VAL	5.0
1	B	210	LEU	5.0
1	A	284	LEU	5.0
1	D	190	LEU	4.9
1	A	208	ILE	4.9
1	C	278	ILE	4.9
1	B	386	ASP	4.9
1	D	211	ASN	4.9
1	B	221	SER	4.8
1	A	211	ASN	4.8
1	D	356	ARG	4.7
1	D	281	ASP	4.7
1	C	333	SER	4.6
1	C	384	PHE	4.5
1	A	188	PRO	4.5
1	C	212	SER	4.5
1	B	334	ASP	4.5
1	C	280	ASN	4.5
1	D	335	GLY	4.4
1	C	332	GLU	4.4
1	D	198	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	284	LEU	4.3
1	D	378	GLY	4.3
1	C	191	THR	4.2
1	C	281	ASP	4.2
1	A	281	ASP	4.2
1	D	213	GLY	4.1
1	A	278	ILE	4.1
1	D	376	ILE	4.1
1	B	279	ASP	4.1
1	C	379	ASP	4.1
1	A	384	PHE	4.1
1	D	191	THR	4.1
1	C	217	ARG	4.1
1	D	284	LEU	4.1
1	C	338	HIS	4.1
1	D	357	GLU	4.1
1	D	202	LEU	4.1
1	D	200	VAL	4.1
1	B	190	LEU	4.0
1	C	382	MET	4.0
1	A	338	HIS	4.0
1	A	294	ASN	3.9
1	A	334	ASP	3.9
1	D	189	ALA	3.9
1	D	333	SER	3.9
1	A	380	SER	3.9
1	B	333	SER	3.8
1	C	380	SER	3.8
1	B	337	GLU	3.8
1	C	357	GLU	3.8
1	C	292	ASP	3.7
1	B	283	GLU	3.7
1	B	387	THR	3.7
1	D	201	LEU	3.7
1	A	378	GLY	3.7
1	B	385	GLY	3.7
1	D	238	GLU	3.7
1	C	378	GLY	3.6
1	B	195	THR	3.6
1	C	190	LEU	3.6
1	D	223	LEU	3.6
1	B	332	GLU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	360	GLU	3.6
1	C	336	LYS	3.6
1	D	395	LEU	3.6
1	D	218	GLU	3.6
1	C	209	SER	3.6
1	C	414	ASP	3.5
1	D	387	THR	3.5
1	C	375	LYS	3.5
1	D	433	ASP	3.5
1	D	219	LEU	3.5
1	D	214	LYS	3.5
1	A	279	ASP	3.5
1	C	365	ASP	3.5
1	D	332	GLU	3.4
1	A	381	CYS	3.4
1	D	280	ASN	3.4
1	A	209	SER	3.4
1	A	332	GLU	3.4
1	D	199	GLU	3.4
1	D	336	LYS	3.4
1	C	385	GLY	3.4
1	D	216	PHE	3.4
1	A	283	GLU	3.4
1	C	205	LYS	3.4
1	B	293	LYS	3.3
1	C	395	LEU	3.3
1	C	203	ASN	3.3
1	B	212	SER	3.3
1	C	202	LEU	3.3
1	D	217	ARG	3.3
1	B	218	GLU	3.3
1	A	336	LYS	3.2
1	D	402	VAL	3.2
1	B	203	ASN	3.2
1	C	291	VAL	3.2
1	C	402	VAL	3.2
1	C	377	VAL	3.1
1	D	192	LYS	3.1
1	A	335	GLY	3.1
1	C	216	PHE	3.1
1	D	434	PHE	3.1
1	D	203	ASN	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	236	ALA	3.1
1	B	338	HIS	3.1
1	B	209	SER	3.1
1	A	203	ASN	3.0
1	D	283	GLU	3.0
1	D	337	GLU	3.0
1	A	379	ASP	3.0
1	A	382	MET	3.0
1	A	293	LYS	3.0
1	D	285	SER	3.0
1	B	288	ILE	3.0
1	D	207	GLU	2.9
1	C	198	LEU	2.9
1	D	388	LEU	2.9
1	B	402	VAL	2.9
1	D	338	HIS	2.9
1	D	188	PRO	2.9
1	A	337	GLU	2.9
1	B	207	GLU	2.9
1	C	337	GLU	2.9
1	C	435	LYS	2.9
1	B	377	VAL	2.9
1	D	195	THR	2.9
1	B	285	SER	2.9
1	D	215	PRO	2.8
1	D	205	LYS	2.8
1	A	212	SER	2.8
1	A	333	SER	2.8
1	B	314	ARG	2.8
1	B	215	PRO	2.8
1	D	386	ASP	2.8
1	B	213	GLY	2.8
1	C	215	PRO	2.8
1	A	435	LYS	2.8
1	B	294	ASN	2.7
1	C	386	ASP	2.7
1	C	192	LYS	2.7
1	D	435	LYS	2.7
1	B	388	LEU	2.7
1	A	205	LYS	2.7
1	A	190	LEU	2.7
1	C	219	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	233	GLN	2.7
1	A	358	ASN	2.7
1	D	369	HIS	2.7
1	A	288	ILE	2.7
1	C	374	PHE	2.7
1	C	188	PRO	2.7
1	A	285	SER	2.7
1	B	335	GLY	2.7
1	C	361	SER	2.6
1	C	195	THR	2.6
1	B	281	ASP	2.6
1	C	394	ASP	2.6
1	D	221	SER	2.6
1	C	211	ASN	2.6
1	D	454	LEU	2.6
1	D	193	SER	2.6
1	A	277	GLY	2.6
1	B	214	LYS	2.6
1	A	386	ASP	2.6
1	D	227	ARG	2.6
1	C	238	GLU	2.5
1	B	284	LEU	2.5
1	C	436	ASN	2.5
1	C	283	GLU	2.5
1	B	200	VAL	2.5
1	D	358	ASN	2.5
1	D	196	ASP	2.5
1	C	387	THR	2.5
1	D	209	SER	2.5
1	D	355	THR	2.5
1	C	356	ARG	2.5
1	B	216	PHE	2.4
1	B	205	LYS	2.4
1	A	387	THR	2.4
1	C	207	GLU	2.4
1	C	218	GLU	2.4
1	A	295	PHE	2.4
1	B	192	LYS	2.3
1	B	336	LYS	2.3
1	A	291	VAL	2.3
1	B	238	GLU	2.3
1	D	377	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	417	TRP	2.3
1	D	224	LEU	2.3
1	C	293	LYS	2.3
1	D	237	GLU	2.3
1	D	194	GLN	2.3
1	C	229	LYS	2.3
1	D	293	LYS	2.3
1	B	357	GLU	2.2
1	B	275	ARG	2.2
1	A	256	ASP	2.2
1	A	385	GLY	2.2
1	C	224	LEU	2.2
1	C	359	LEU	2.2
1	C	233	GLN	2.2
1	D	292	ASP	2.2
1	A	359	LEU	2.2
1	B	260	LEU	2.2
1	B	291	VAL	2.2
1	D	291	VAL	2.2
1	A	213	GLY	2.2
1	D	449	GLY	2.2
1	A	287	GLN	2.2
1	A	388	LEU	2.2
1	C	201	LEU	2.2
1	D	445	SER	2.2
1	D	206	ASP	2.2
1	C	362	ILE	2.1
1	C	376	ILE	2.1
1	B	287	GLN	2.1
1	C	287	GLN	2.1
1	C	388	LEU	2.1
1	D	225	SER	2.1
1	A	195	THR	2.1
1	C	363	ILE	2.1
1	D	197	ARG	2.1
1	B	202	LEU	2.1
1	A	280	ASN	2.1
1	D	365	ASP	2.1
1	C	413	ILE	2.1
1	D	413	ILE	2.1
1	B	222	GLU	2.1
1	A	207	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	220	GLU	2.0
1	D	361	SER	2.1
1	B	231	LEU	2.0
1	B	409	ARG	2.0
1	C	214	LYS	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](#)

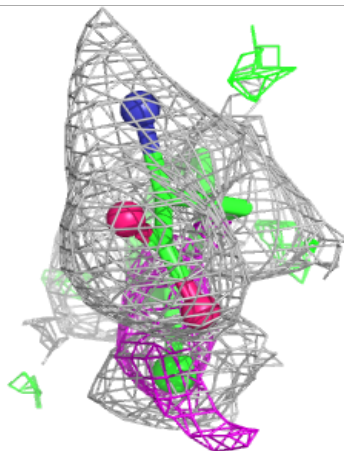
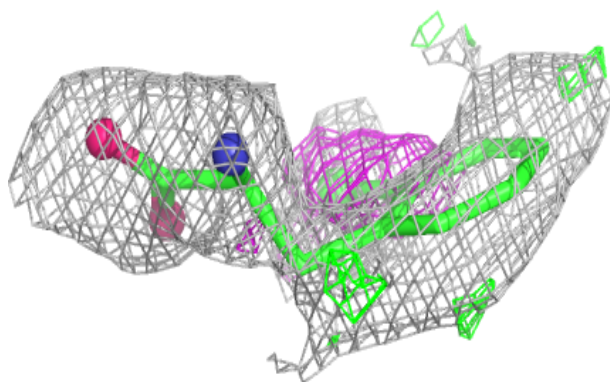
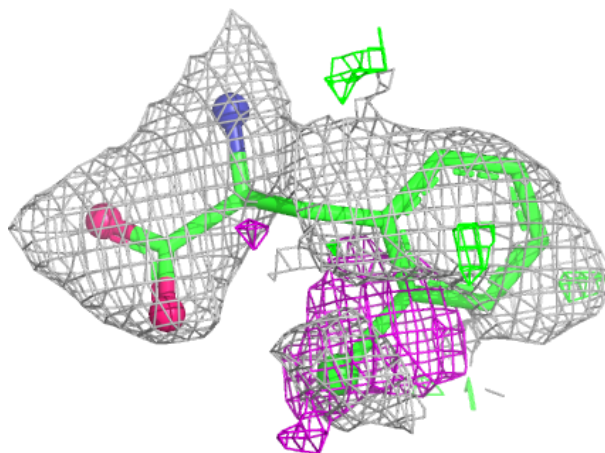
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	2L5	C	502	13/13	0.66	0.21	40,43,49,53	0
3	2L5	A	502	13/13	0.72	0.19	37,42,49,53	0
3	2L5	D	502	13/13	0.75	0.17	37,42,49,54	0
3	2L5	B	502	13/13	0.76	0.18	38,46,54,56	0
2	ANP	A	501	31/31	0.85	0.14	33,42,62,71	0
2	ANP	C	501	31/31	0.85	0.13	37,46,62,75	0
2	ANP	D	501	31/31	0.89	0.12	37,43,60,63	0
2	ANP	B	501	31/31	0.90	0.11	32,39,59,69	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.

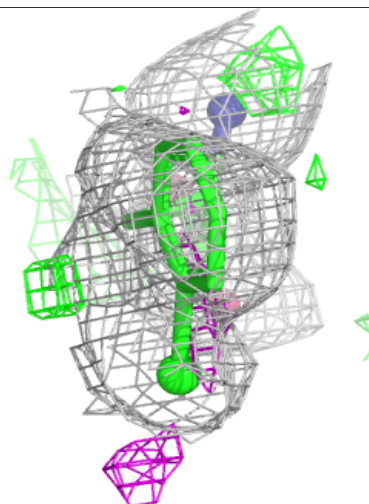
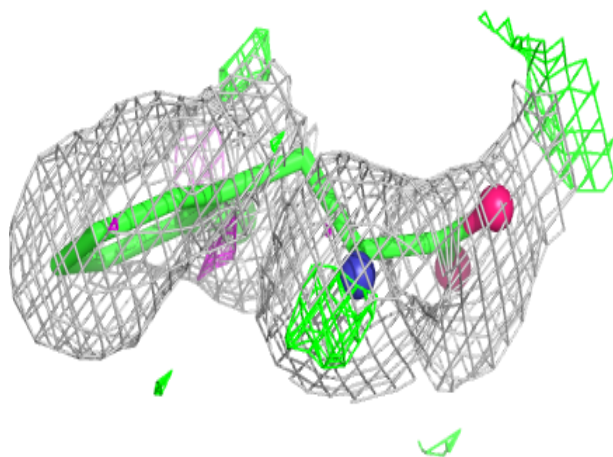
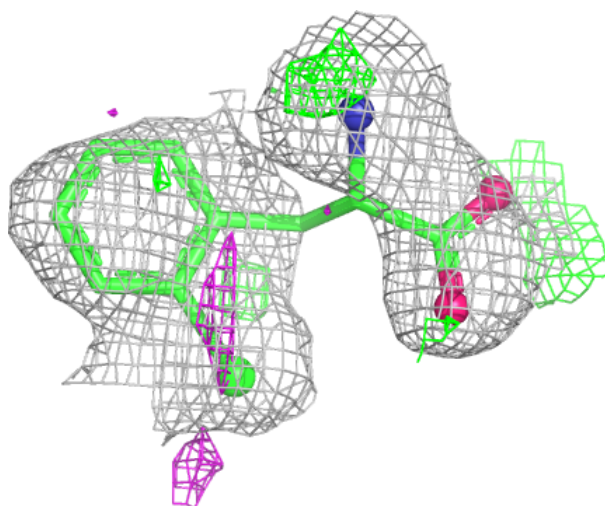
Electron density around 2L5 C 502:

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



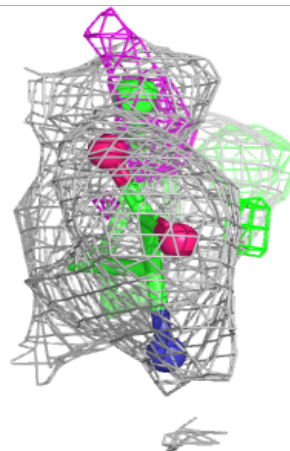
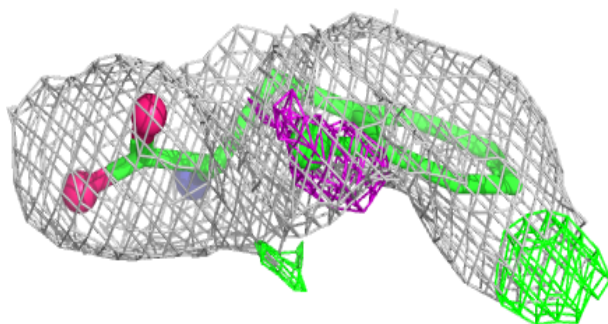
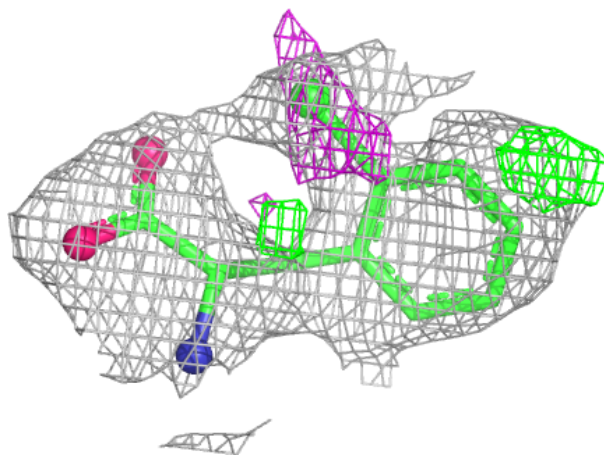
Electron density around 2L5 A 502:

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



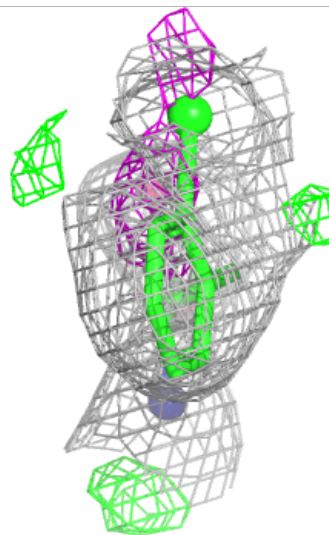
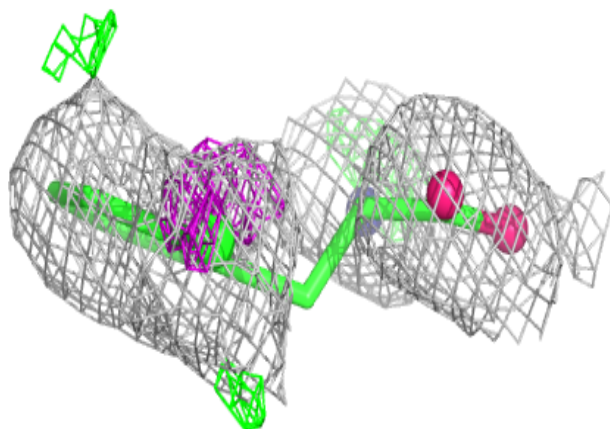
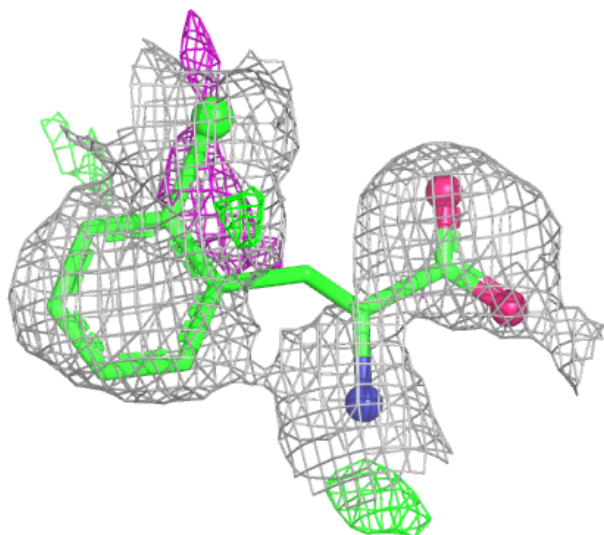
Electron density around 2L5 D 502:

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



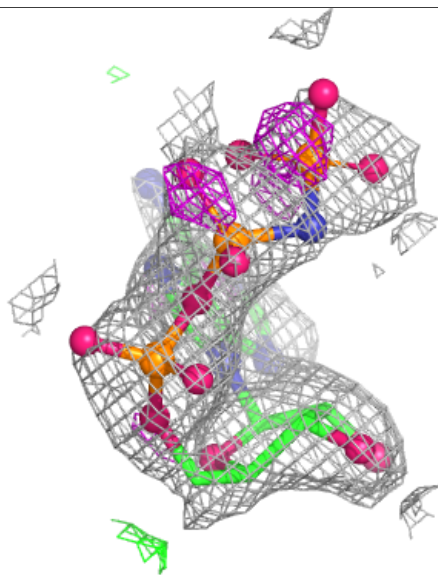
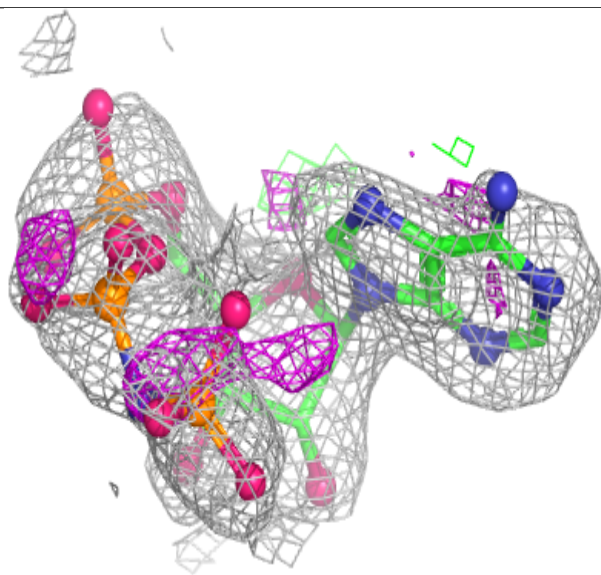
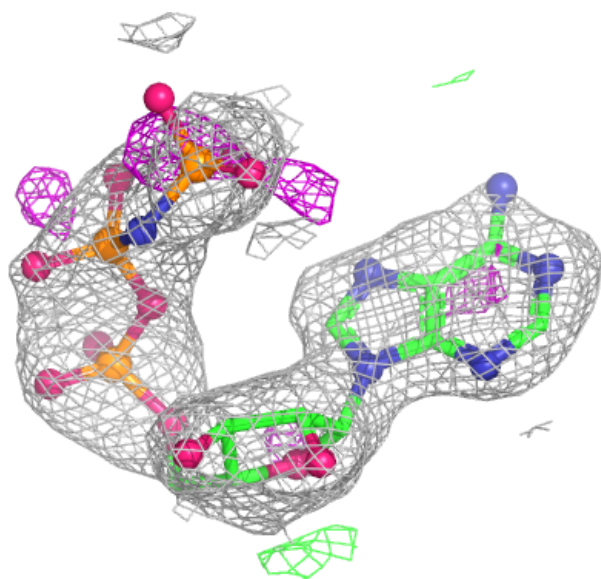
Electron density around 2L5 B 502:

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



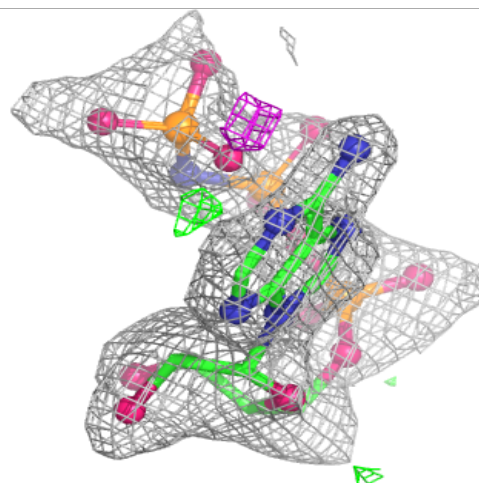
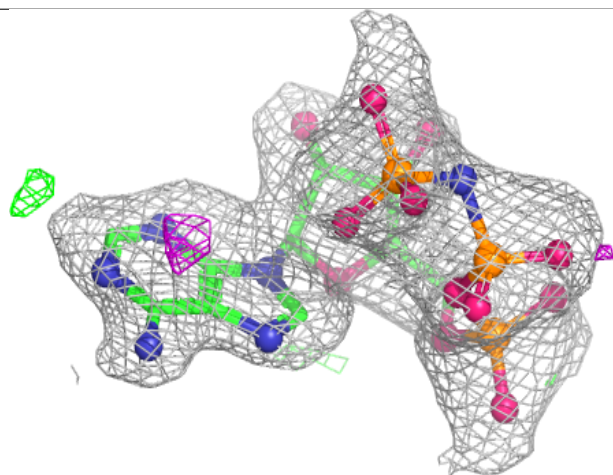
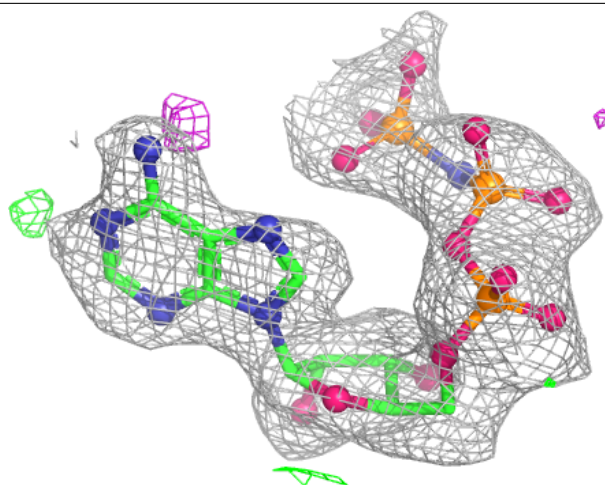
Electron density around ANP A 501:

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



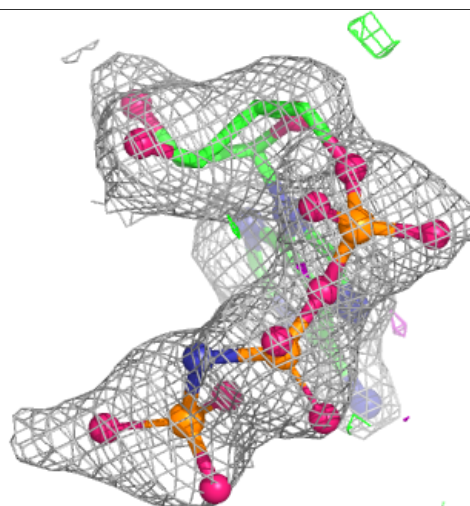
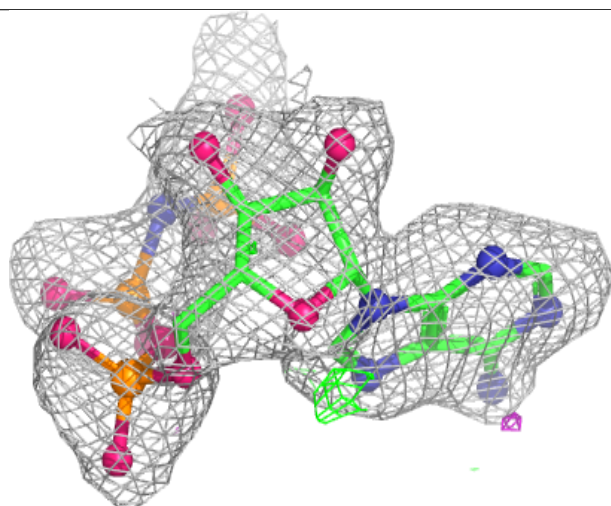
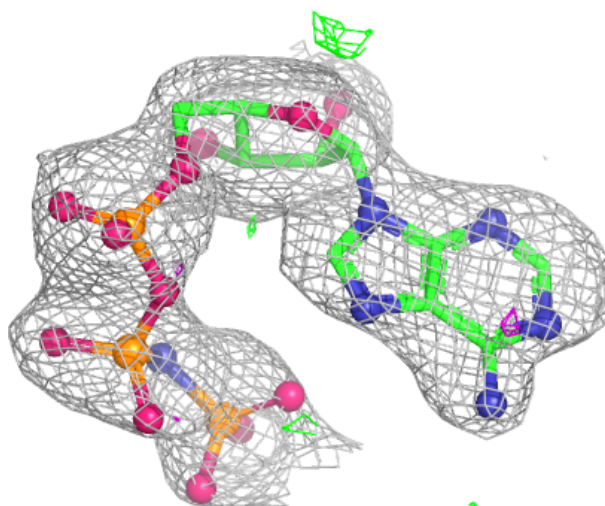
Electron density around ANP C 501:

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



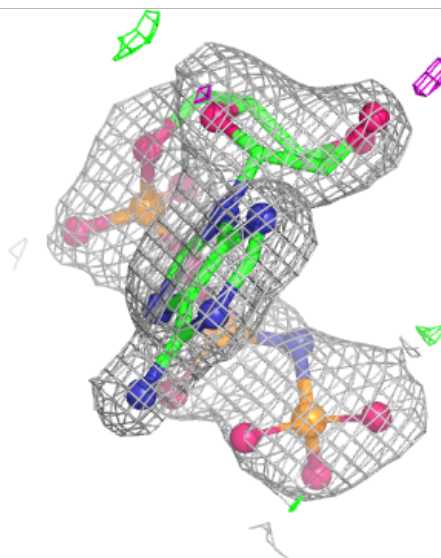
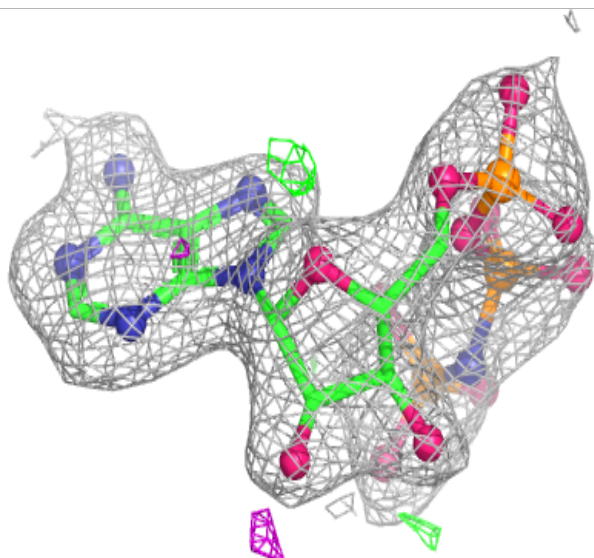
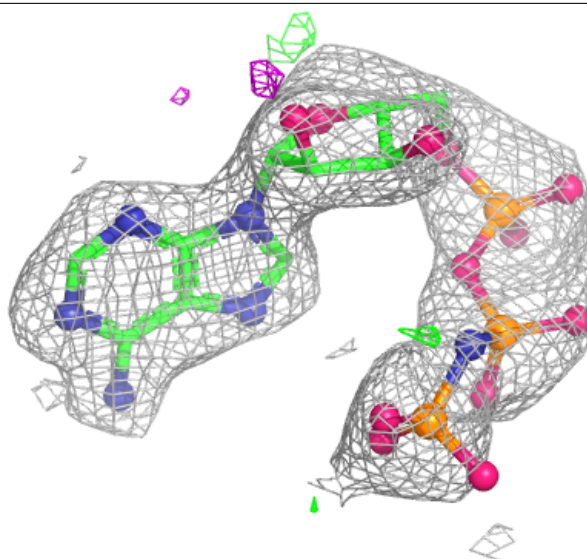
Electron density around ANP D 501:

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



Electron density around ANP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.