



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2022 – 12:07 PM EDT

PDB ID : 7RSM
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

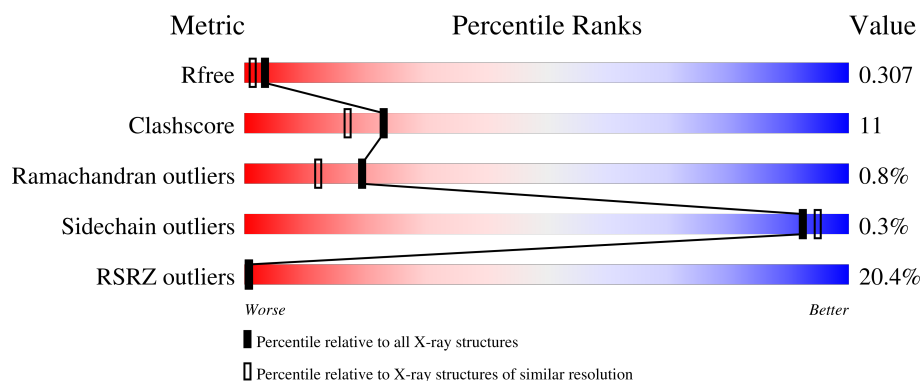
1 Overall quality at a glance

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}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (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	<div> <div>16%</div> <div>82%</div> <div>17%</div> </div>
1	B	267	<div> <div>21%</div> <div>73%</div> <div>25%</div> </div>
1	C	267	<div> <div>22%</div> <div>76%</div> <div>22%</div> </div>
1	D	267	<div> <div>23%</div> <div>80%</div> <div>19%</div> </div>

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:

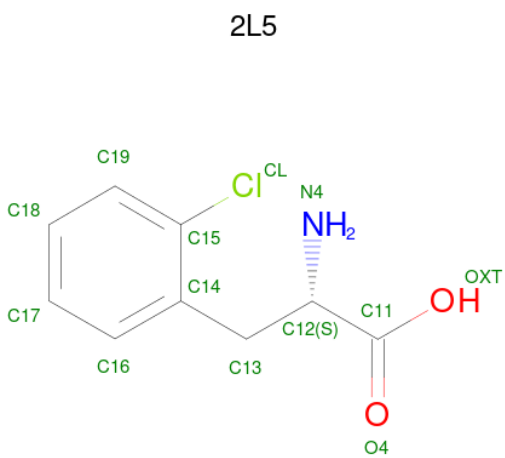
Chain	Residue	Modelled	Actual	Comment	Reference
A	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
A	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
A	384	PHE	TYR	engineered mutation	UNP A0A0F8JXW8
B	346	ASP	ASN	engineered mutation	UNP A0A0F8JXW8
B	348	SER	CYS	engineered mutation	UNP A0A0F8JXW8
B	384	PHE	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 (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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 (three-letter code: 2L5) (formula: $\text{C}_9\text{H}_9\text{ClNO}_2$) (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

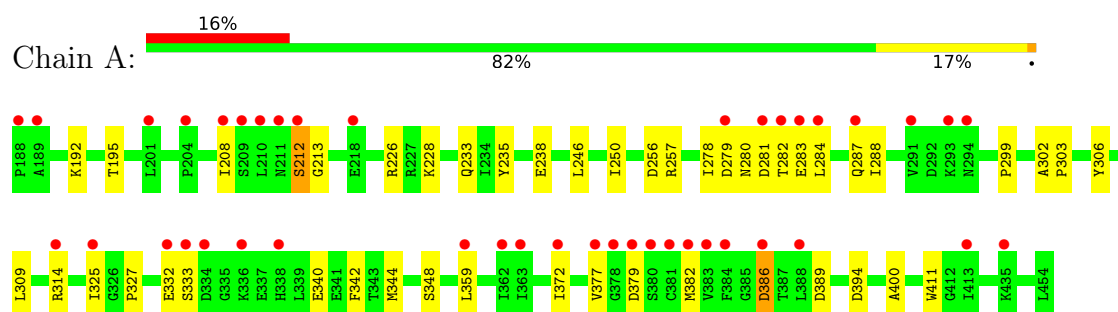
- Molecule 4 is water.

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

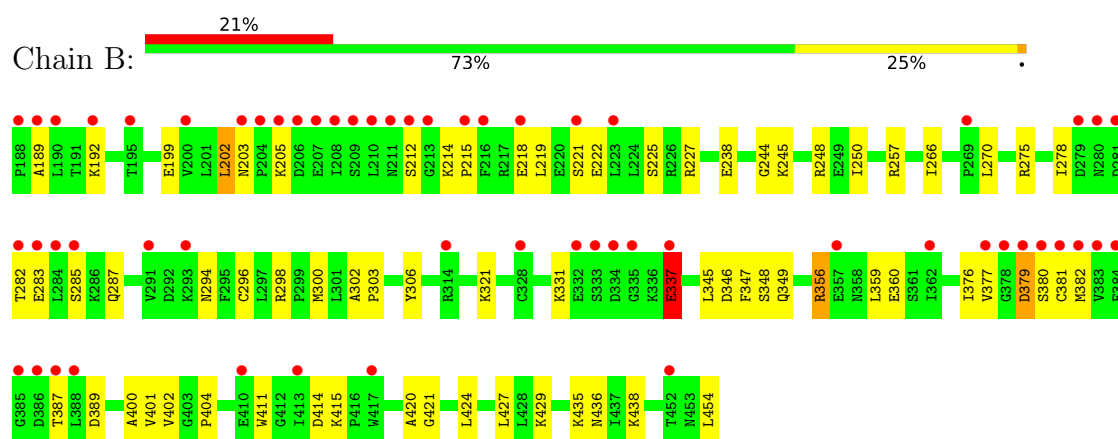
3 Residue-property plots [i](#)

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.

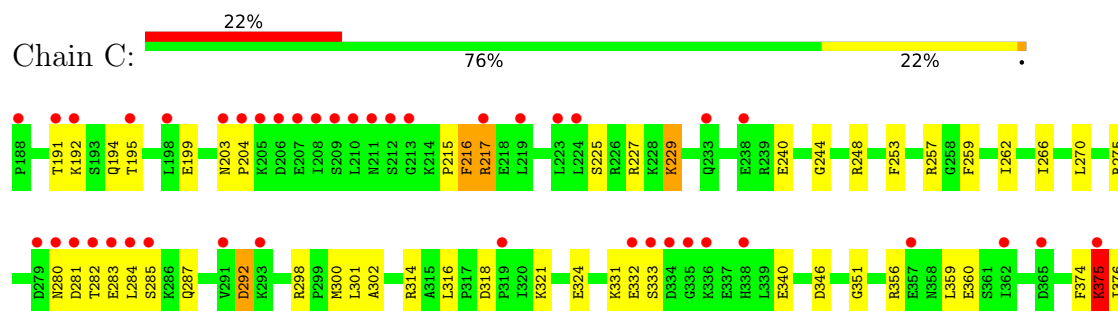
• Molecule 1: Pyrrolysine-tRNA ligase

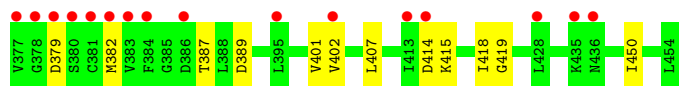


• Molecule 1: Pyrrolysine-tRNA ligase

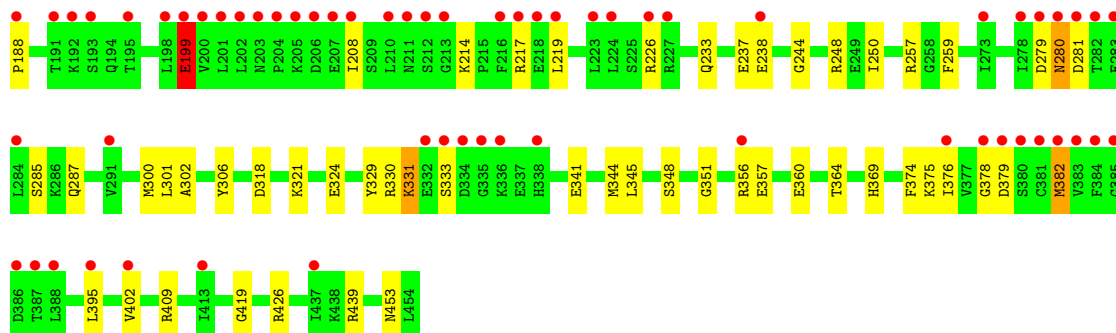
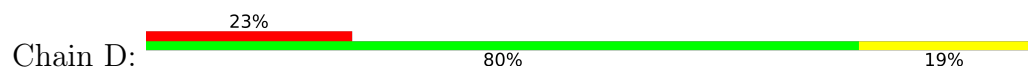


• Molecule 1: Pyrrolysine-tRNA ligase





● 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	3275 reflections (5.15%)	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 , 50.2	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	0.92	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	0.52	0/2210	0.74	2/2972 (0.1%)
1	B	0.52	0/2210	0.74	3/2972 (0.1%)
1	C	0.62	3/2210 (0.1%)	0.86	8/2972 (0.3%)
1	D	0.57	3/2210 (0.1%)	0.98	4/2972 (0.1%)
All	All	0.56	6/8840 (0.1%)	0.84	17/11888 (0.1%)

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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	375	LYS	CD-CE	14.98	1.88	1.51
1	D	199	GLU	CD-OE2	9.67	1.36	1.25
1	D	199	GLU	CD-OE1	5.38	1.31	1.25
1	D	199	GLU	CG-CD	-5.34	1.44	1.51
1	C	375	LYS	CG-CD	5.26	1.70	1.52
1	C	217	ARG	CB-CG	-5.18	1.38	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	GLU	OE1-CD-OE2	-24.82	93.52	123.30
1	D	199	GLU	CG-CD-OE1	21.97	162.24	118.30
1	C	375	LYS	CG-CD-CE	-18.09	57.64	111.90
1	D	199	GLU	CG-CD-OE2	-16.01	86.29	118.30
1	C	217	ARG	CG-CD-NE	-10.65	89.43	111.80
1	C	375	LYS	CB-CA-C	7.84	126.09	110.40
1	A	386	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	C	292	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	B	356	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	D	257	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	B	202	LEU	C-N-CA	5.76	136.10	121.70
1	C	375	LYS	CA-CB-CG	-5.59	101.10	113.40
1	C	229	LYS	CB-CG-CD	5.22	125.18	111.60
1	A	257	ARG	CA-C-N	5.20	126.60	116.20
1	B	337	GLU	CG-CD-OE2	-5.09	108.12	118.30
1	C	217	ARG	CB-CG-CD	5.08	124.82	111.60
1	C	375	LYS	N-CA-CB	-5.08	101.45	110.60

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	39	1
1	B	2168	0	2175	69	2
1	C	2168	0	2175	49	1
1	D	2168	0	2175	49	1
2	A	31	0	13	0	0
2	B	31	0	13	0	0
2	C	31	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	31	0	13	0	0
3	A	13	0	9	9	0
3	B	13	0	9	10	0
3	C	13	0	9	4	0
3	D	13	0	9	10	0
4	A	100	0	0	6	0
4	B	89	0	0	11	2
4	C	61	0	0	1	0
4	D	83	0	0	15	2
All	All	9181	0	8788	201	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 11.

All (201) 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: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
1:D:375:LYS:NZ	4:D:603:HOH:O	2.01	0.76
1:D:238:GLU:C	4:D:604:HOH:O	2.24	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ARG:NH2	1:B:379:ASP:O	2.17	0.70
1:B:214:LYS:HE2	1:B:219:LEU:HD21	1.74	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: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: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: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:D:302:ALA:HB2	3:D:502:2L5:H5	1.81	0.61
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:415:LYS:NZ	4:B:605:HOH:O	2.09	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
1:C:284:LEU:HD21	1:C:300:MET:HE1	1.85	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: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:B:429:LYS:NZ	4:B:615:HOH:O	2.38	0.56
1:C:302:ALA:HB2	3:C:502:2L5:H5	1.89	0.55
1:C:194:GLN:HG2	1:C:216:PHE:CD2	2.42	0.55
1:A:359:LEU:HD21	1:A:400:ALA:HB1	1.89	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:ALA:H	1:C:281:ASP:CG	2.12	0.53
1:B:356:ARG:HH12	1:B:379:ASP:HB3	1.73	0.53
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:A:279:ASP:C	1:A:281:ASP:H	2.13	0.52
1:A:302:ALA:CB	3:A:502:2L5:H4	2.39	0.51
1:B:379:ASP:HB2	1:B:382:MET:HE3	1.92	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:A:302:ALA:HB2	3:A:502:2L5:H5	1.93	0.50
1:B:266:ILE:HA	1:B:298:ARG:HD3	1.92	0.50
1:C:215:PRO:C	1:C:217:ARG:H	2.15	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:374:PHE:C	1:D:375:LYS:HD3	2.32	0.50
1:D:287:GLN:HA	1:D:331:LYS:HB2	1.94	0.50
1:D:360:GLU:O	1:D:364:THR:OG1	2.25	0.50
1:D:279:ASP:C	1:D:281:ASP:H	2.15	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:356:ARG:HH22	1:B:379:ASP:C	2.10	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:D:300:MET:HA	1:D:344:MET:HE3	1.96	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:C:215:PRO:C	1:C:217:ARG:N	2.68	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: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: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
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
3:D:502:2L5:N4	4:D:607:HOH:O	2.25	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
1:D:287:GLN:NE2	1:D:330:ARG:HB3	2.33	0.42
1:B:199:GLU:O	1:B:435:LYS:NZ	2.48	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:A:394:ASP:CG	4:A:602:HOH:O	2.55	0.41
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:B:377:VAL:CG2	1:B:389:ASP:HB2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:THR:HG22	1:C:194:GLN:CD	2.42	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 [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	265/267 (99%)	249 (94%)	13 (5%)	3 (1%)	14	8
1	B	265/267 (99%)	241 (91%)	24 (9%)	0	100	100
1	C	265/267 (99%)	249 (94%)	14 (5%)	2 (1%)	19	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	265/267 (99%)	246 (93%)	16 (6%)	3 (1%)	14	8
All	All	1060/1068 (99%)	985 (93%)	67 (6%)	8 (1%)	19	12

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%)	239 (99%)	2 (1%)	81	86
1	C	241/241 (100%)	240 (100%)	1 (0%)	91	93
1	D	241/241 (100%)	241 (100%)	0	100	100
All	All	964/964 (100%)	961 (100%)	3 (0%)	92	95

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

Mol	Chain	Res	Type
1	B	221	SER
1	B	379	ASP
1	C	375	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	HIS
1	C	194	GLN
1	C	233	GLN
1	C	280	ASN
1	C	368	ASN
1	D	287	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	502	-	12,13,13	1.02	1 (8%)	14,17,17	1.22	2 (14%)
2	ANP	C	501	-	29,33,33	1.22	4 (13%)	31,52,52	1.02	3 (9%)
2	ANP	A	501	-	29,33,33	1.23	5 (17%)	31,52,52	1.20	4 (12%)
3	2L5	B	502	-	12,13,13	0.99	1 (8%)	14,17,17	0.76	0
2	ANP	D	501	-	29,33,33	1.22	4 (13%)	31,52,52	1.01	3 (9%)
2	ANP	B	501	-	29,33,33	1.24	5 (17%)	31,52,52	1.12	3 (9%)
3	2L5	D	502	-	12,13,13	1.17	1 (8%)	14,17,17	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	2L5	C	502	-	12,13,13	1.11	1 (8%)	14,17,17	0.97	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	2L5	A	502	-	-	1/8/8/8	0/1/1/1
2	ANP	C	501	-	-	7/14/38/38	0/3/3/3
2	ANP	A	501	-	-	7/14/38/38	0/3/3/3
3	2L5	B	502	-	-	1/8/8/8	0/1/1/1
2	ANP	D	501	-	-	7/14/38/38	0/3/3/3
2	ANP	B	501	-	-	4/14/38/38	0/3/3/3
3	2L5	D	502	-	-	4/8/8/8	0/1/1/1
3	2L5	C	502	-	-	4/8/8/8	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	ANP	PG-O1G	3.13	1.51	1.46
3	D	502	2L5	C15-CL	3.02	1.80	1.73
2	D	501	ANP	PG-N3B	3.01	1.71	1.63
2	A	501	ANP	PB-O1B	3.00	1.50	1.46
2	A	501	ANP	PG-N3B	2.97	1.71	1.63
2	A	501	ANP	PG-O1G	2.91	1.50	1.46
3	C	502	2L5	C15-CL	2.90	1.80	1.73
2	C	501	ANP	PG-N3B	2.90	1.70	1.63
2	B	501	ANP	PG-O1G	2.89	1.50	1.46
2	B	501	ANP	PB-O1B	2.86	1.50	1.46
2	D	501	ANP	PG-O1G	2.82	1.50	1.46
2	B	501	ANP	PG-N3B	2.81	1.70	1.63
2	D	501	ANP	PB-O1B	2.79	1.50	1.46
2	C	501	ANP	PB-O1B	2.67	1.50	1.46
2	B	501	ANP	PB-O3A	-2.52	1.55	1.59
2	D	501	ANP	PB-N3B	2.47	1.69	1.63
3	A	502	2L5	C15-CL	2.37	1.79	1.73
2	C	501	ANP	PB-N3B	2.34	1.69	1.63
3	B	502	2L5	C15-CL	2.15	1.78	1.73
2	A	501	ANP	PB-N3B	2.14	1.69	1.63
2	A	501	ANP	PB-O3A	-2.11	1.56	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	ANP	PB-N3B	2.10	1.68	1.63

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	ANP	PB-O3A-PA	-3.21	121.30	132.62
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	-2.52	107.12	113.45
2	C	501	ANP	PB-O3A-PA	-2.49	123.86	132.62
2	C	501	ANP	O1B-PB-N3B	-2.47	108.14	111.77
3	A	502	2L5	C14-C15-CL	-2.36	115.89	119.73
2	A	501	ANP	C5-C6-N6	2.35	123.92	120.35
2	B	501	ANP	PB-O3A-PA	-2.30	124.53	132.62
2	B	501	ANP	C5-C6-N6	2.20	123.70	120.35
2	A	501	ANP	O2G-PG-O1G	-2.20	107.93	113.45
2	D	501	ANP	C5-C6-N6	2.11	123.55	120.35
3	A	502	2L5	C19-C15-CL	2.05	122.52	118.41
2	D	501	ANP	O2G-PG-O1G	-2.05	108.31	113.45
2	A	501	ANP	O3G-PG-O1G	-2.01	108.39	113.45

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	ANP	PB-N3B-PG-O1G
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	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-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
3	C	502	2L5	C11-C12-C13-C14
3	D	502	2L5	C11-C12-C13-C14
3	D	502	2L5	N4-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
3	D	502	2L5	OXT-C11-C12-C13
2	A	501	ANP	C5'-O5'-PA-O3A
2	C	501	ANP	C5'-O5'-PA-O3A
2	A	501	ANP	C5'-O5'-PA-O1A
2	C	501	ANP	C5'-O5'-PA-O1A
2	C	501	ANP	PG-N3B-PB-O3A
3	D	502	2L5	O4-C11-C12-C13
3	B	502	2L5	C11-C12-C13-C14
3	C	502	2L5	N4-C12-C13-C14
2	B	501	ANP	C4'-C5'-O5'-PA
3	C	502	2L5	O4-C11-C12-C13
3	C	502	2L5	OXT-C11-C12-C13
2	A	501	ANP	C4'-C5'-O5'-PA
2	C	501	ANP	PG-N3B-PB-O1B
2	C	501	ANP	C4'-C5'-O5'-PA
3	A	502	2L5	C11-C12-C13-C14
2	D	501	ANP	C5'-O5'-PA-O3A
2	B	501	ANP	C5'-O5'-PA-O1A

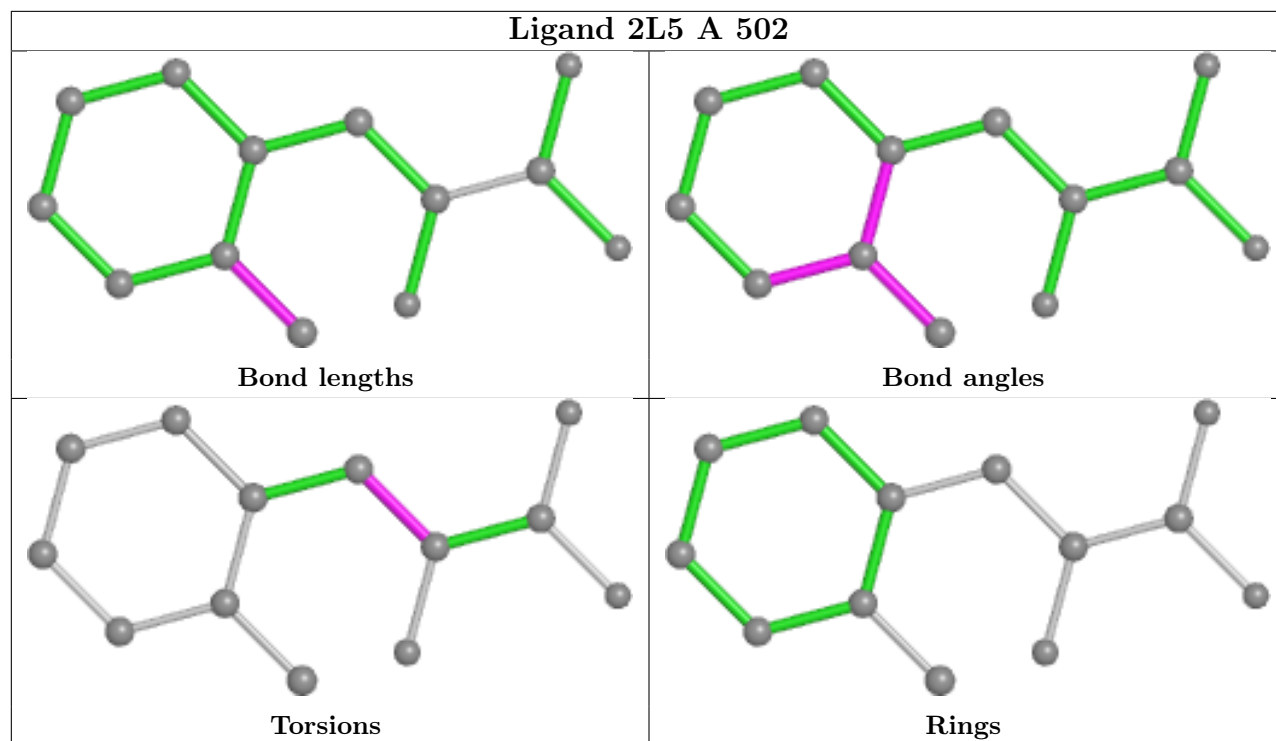
There are no ring outliers.

4 monomers are involved in 33 short contacts:

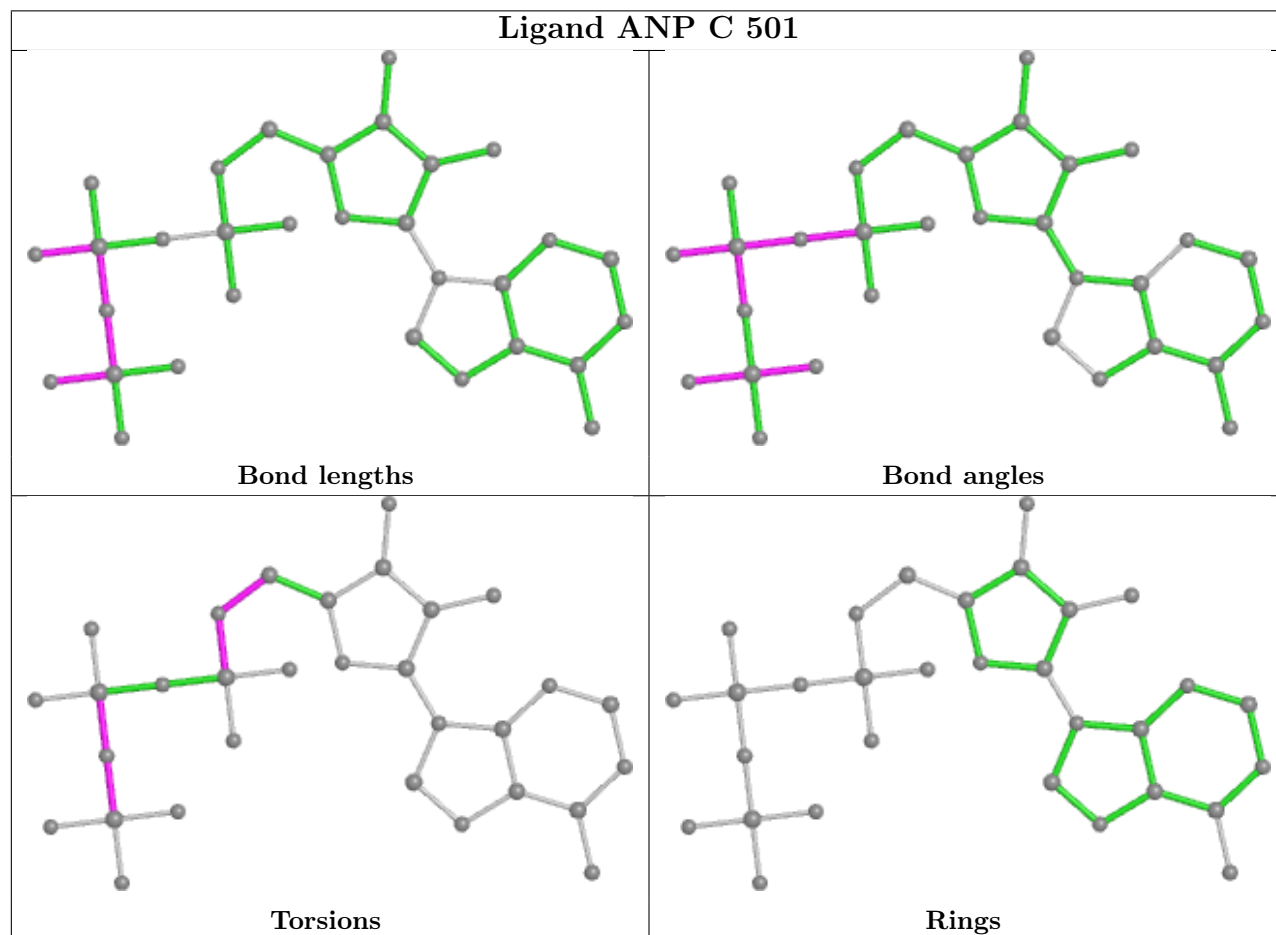
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	2L5	9	0
3	B	502	2L5	10	0
3	D	502	2L5	10	0
3	C	502	2L5	4	0

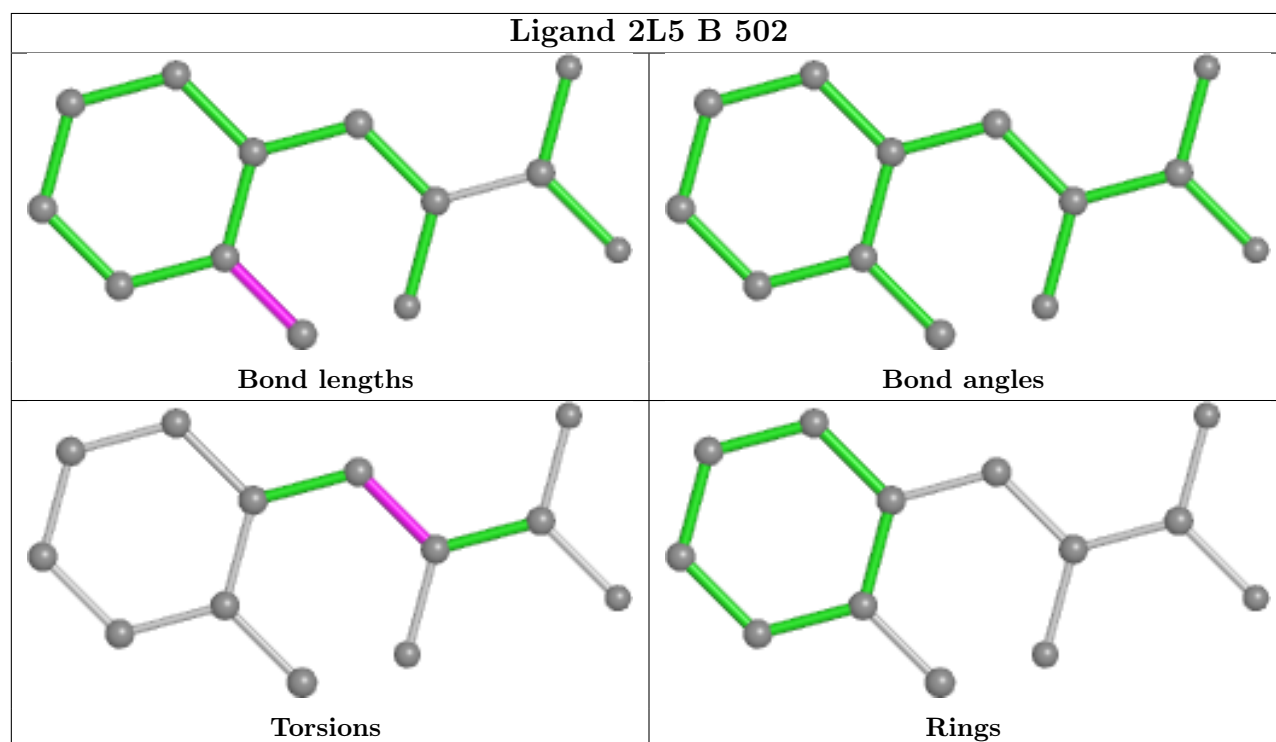
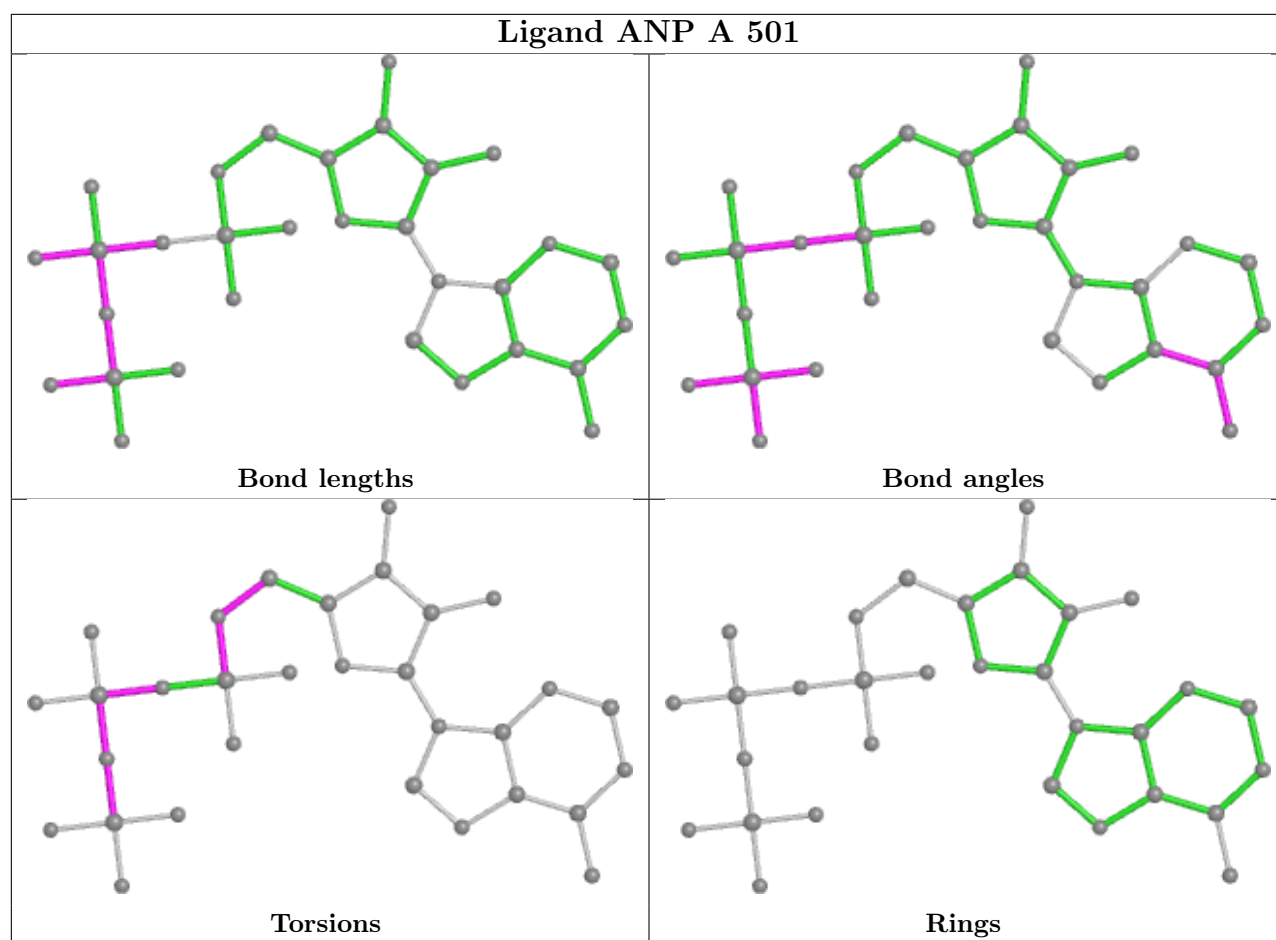
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

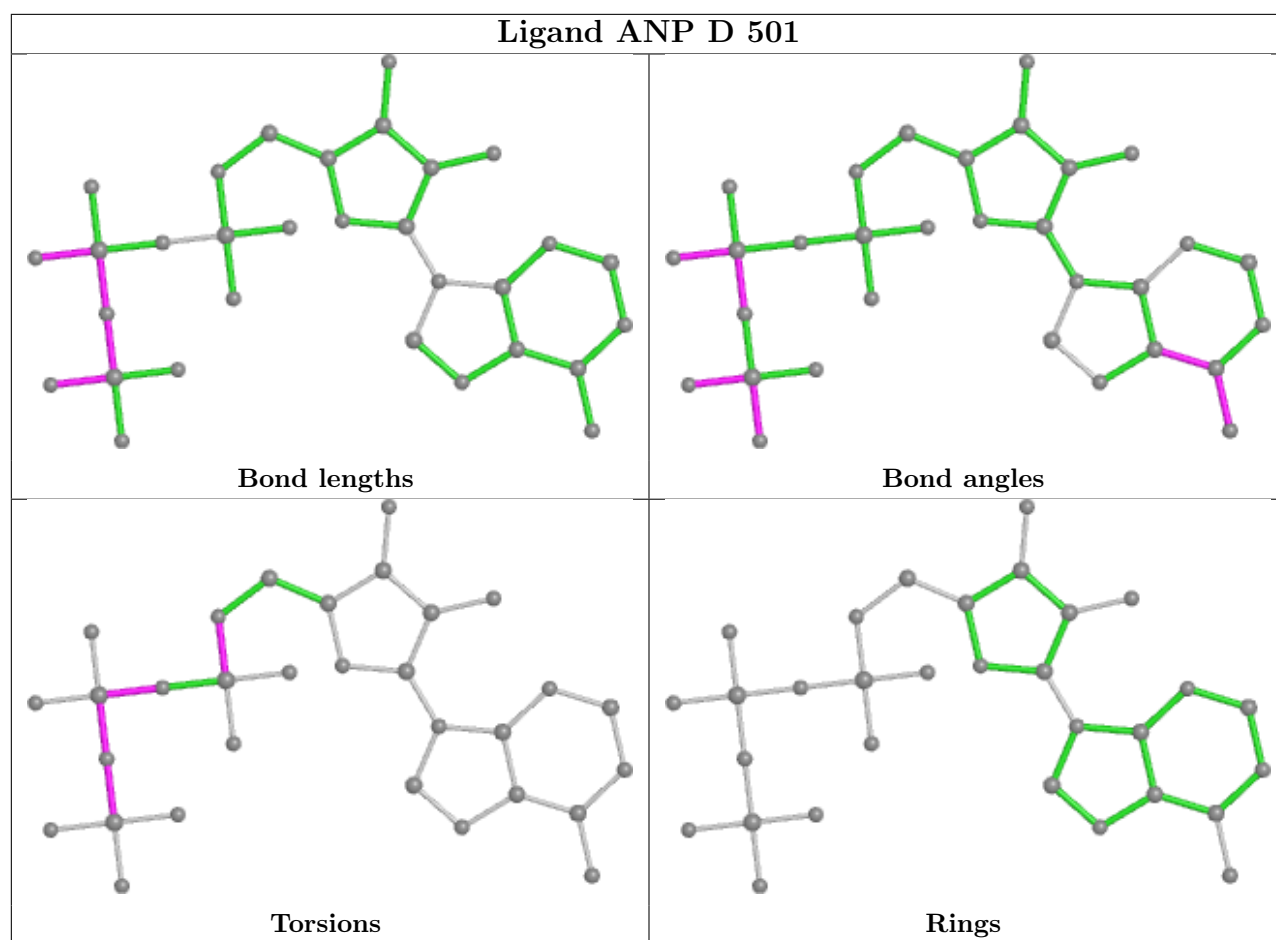
Ligand 2L5 A 502

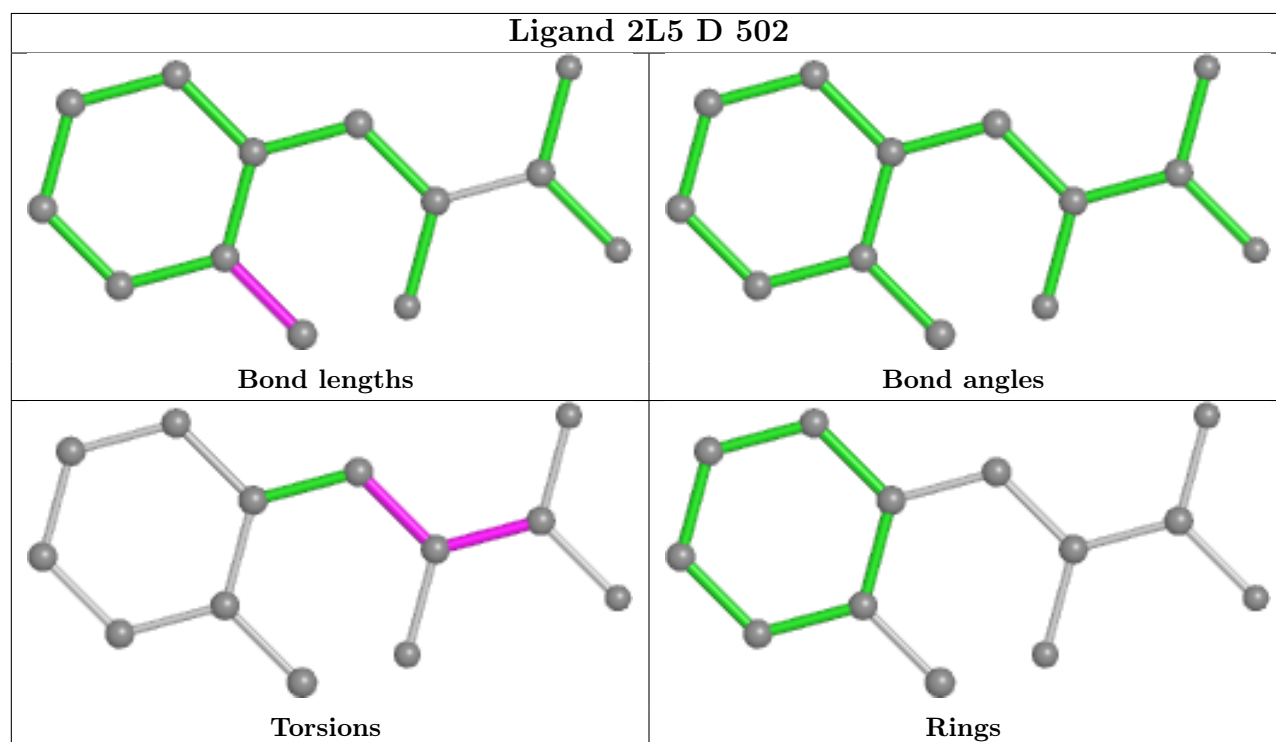
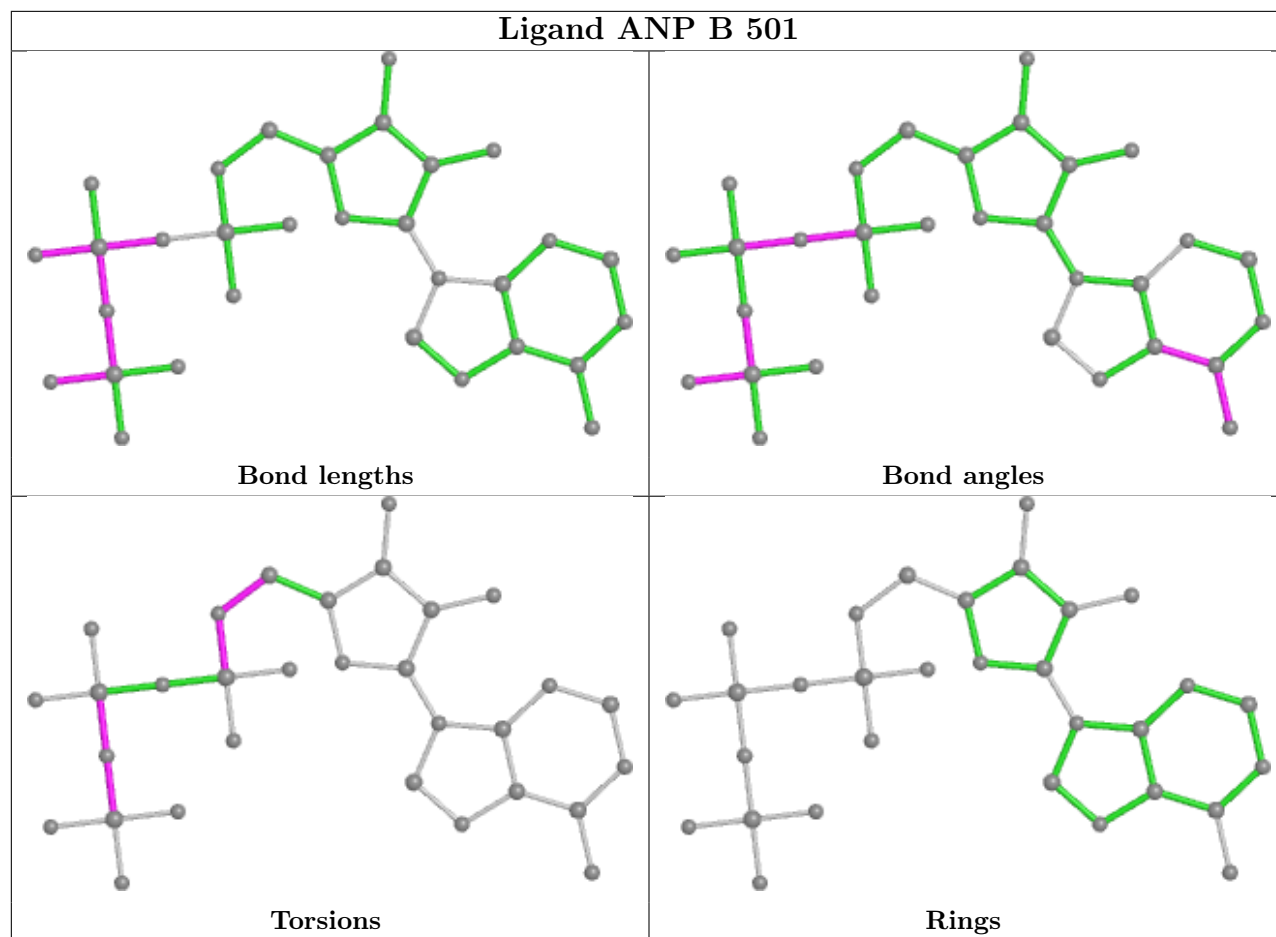


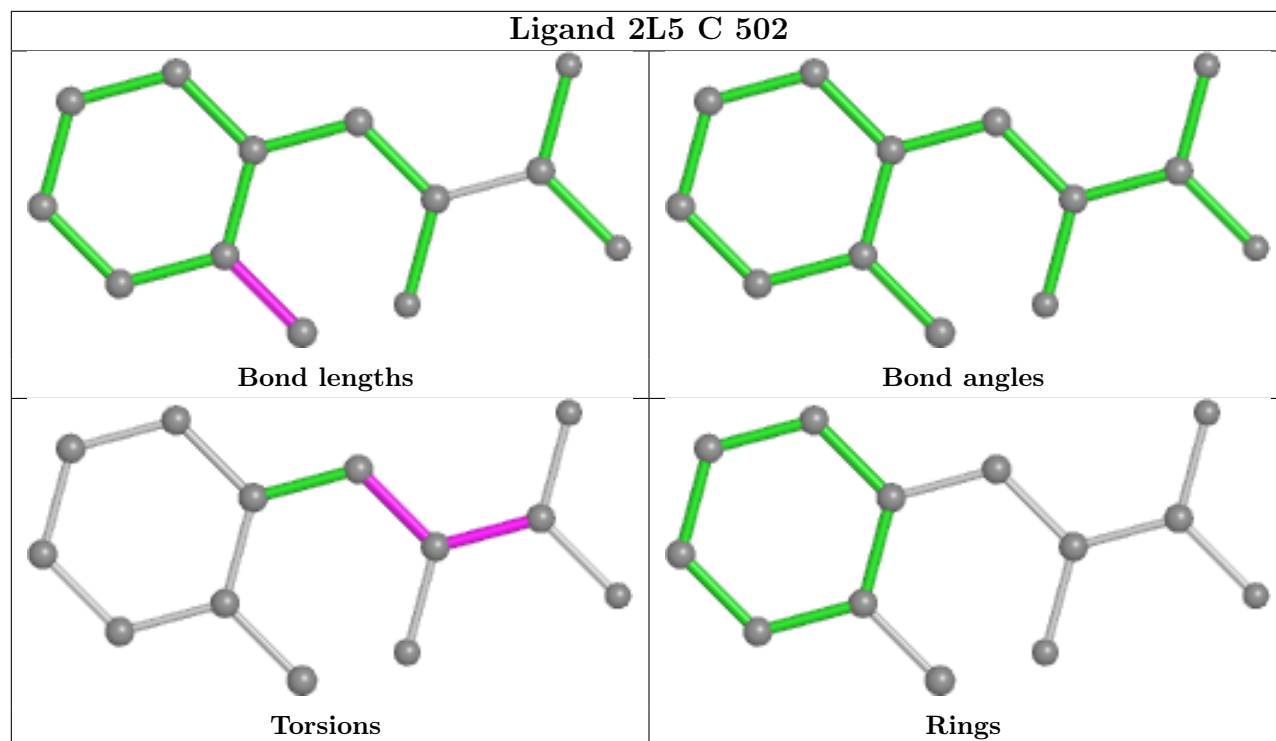
Ligand ANP C 501











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/267 (100%)	1.31	42 (15%) 2 2	22, 35, 77, 99	0
1	B	267/267 (100%)	1.65	57 (21%) 0 0	21, 38, 83, 97	0
1	C	267/267 (100%)	1.52	58 (21%) 0 0	22, 39, 86, 103	0
1	D	267/267 (100%)	1.66	61 (22%) 0 0	22, 39, 86, 99	0
All	All	1068/1068 (100%)	1.53	218 (20%) 1 1	21, 38, 82, 103	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	SER	17.8
1	C	279	ASP	13.0
1	B	379	ASP	11.9
1	D	279	ASP	11.9
1	B	381	CYS	11.8
1	D	382	MET	11.8
1	D	281	ASP	11.7
1	C	210	LEU	11.5
1	D	381	CYS	11.4
1	B	384	PHE	11.3
1	C	381	CYS	10.9
1	A	210	LEU	10.9
1	A	211	ASN	10.6
1	D	380	SER	10.5
1	A	282	THR	10.5
1	B	383	VAL	10.2
1	B	282	THR	9.6
1	D	334	ASP	9.4
1	B	334	ASP	9.4
1	B	211	ASN	9.2
1	D	212	SER	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	381	CYS	8.8
1	B	210	LEU	8.6
1	C	281	ASP	8.5
1	D	383	VAL	8.3
1	C	282	THR	7.9
1	C	379	ASP	7.9
1	C	204	PRO	7.6
1	B	188	PRO	7.4
1	D	207	GLU	7.3
1	B	281	ASP	7.1
1	A	334	ASP	7.1
1	B	386	ASP	7.0
1	C	208	ILE	6.9
1	A	281	ASP	6.8
1	D	385	GLY	6.7
1	D	211	ASN	6.7
1	B	189	ALA	6.6
1	D	282	THR	6.6
1	A	209	SER	6.2
1	A	188	PRO	6.2
1	D	208	ILE	6.0
1	C	334	ASP	6.0
1	C	211	ASN	6.0
1	B	382	MET	5.9
1	D	204	PRO	5.8
1	B	333	SER	5.8
1	C	382	MET	5.6
1	B	204	PRO	5.5
1	B	279	ASP	5.5
1	C	207	GLU	5.5
1	A	279	ASP	5.3
1	D	379	ASP	5.3
1	B	378	GLY	5.3
1	B	283	GLU	5.3
1	C	212	SER	5.1
1	B	212	SER	5.1
1	C	384	PHE	5.1
1	C	283	GLU	5.0
1	C	380	SER	4.9
1	C	209	SER	4.8
1	D	213	GLY	4.8
1	C	213	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	384	PHE	4.7
1	D	238	GLU	4.5
1	A	383	VAL	4.5
1	A	384	PHE	4.4
1	C	383	VAL	4.4
1	D	193	SER	4.2
1	D	210	LEU	4.2
1	C	335	GLY	4.2
1	C	333	SER	4.1
1	A	189	ALA	4.1
1	B	413	ILE	4.0
1	A	204	PRO	4.0
1	D	402	VAL	3.9
1	C	435	LYS	3.9
1	C	332	GLU	3.8
1	D	356	ARG	3.8
1	C	280	ASN	3.8
1	D	192	LYS	3.7
1	D	205	LYS	3.7
1	D	280	ASN	3.7
1	B	377	VAL	3.7
1	A	283	GLU	3.7
1	A	380	SER	3.7
1	A	378	GLY	3.7
1	D	219	LEU	3.6
1	D	395	LEU	3.6
1	B	293	LYS	3.6
1	C	395	LEU	3.5
1	B	209	SER	3.5
1	B	410	GLU	3.4
1	D	336	LYS	3.4
1	D	198	LEU	3.4
1	C	192	LYS	3.4
1	C	291	VAL	3.4
1	A	208	ILE	3.4
1	D	333	SER	3.4
1	D	332	GLU	3.4
1	B	385	GLY	3.4
1	A	382	MET	3.3
1	D	378	GLY	3.3
1	C	188	PRO	3.3
1	B	207	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	452	THR	3.3
1	C	402	VAL	3.3
1	C	217	ARG	3.3
1	D	376	ILE	3.3
1	D	218	GLU	3.2
1	C	223	LEU	3.2
1	B	218	GLU	3.1
1	B	208	ILE	3.1
1	C	377	VAL	3.1
1	D	413	ILE	3.1
1	A	284	LEU	3.1
1	C	338	HIS	3.0
1	C	205	LYS	3.0
1	A	294	ASN	3.0
1	D	291	VAL	3.0
1	B	387	THR	3.0
1	B	280	ASN	3.0
1	C	336	LYS	3.0
1	A	379	ASP	2.9
1	C	357	GLU	2.9
1	D	191	THR	2.9
1	C	203	ASN	2.9
1	C	378	GLY	2.9
1	D	216	PHE	2.9
1	A	293	LYS	2.9
1	B	221	SER	2.9
1	A	291	VAL	2.8
1	A	333	SER	2.8
1	C	375	LYS	2.8
1	D	278	ILE	2.8
1	C	219	LEU	2.8
1	D	283	GLU	2.7
1	B	203	ASN	2.7
1	D	273	ILE	2.7
1	B	205	LYS	2.6
1	B	285	SER	2.6
1	B	195	THR	2.6
1	D	227	ARG	2.6
1	D	195	THR	2.6
1	A	386	ASP	2.6
1	D	223	LEU	2.6
1	A	388	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	284	LEU	2.6
1	C	233	GLN	2.5
1	D	224	LEU	2.5
1	A	212	SER	2.5
1	C	428	LEU	2.5
1	A	435	LYS	2.5
1	B	337	GLU	2.5
1	C	284	LEU	2.4
1	D	201	LEU	2.4
1	C	206	ASP	2.4
1	C	195	THR	2.4
1	B	332	GLU	2.4
1	D	388	LEU	2.4
1	C	238	GLU	2.4
1	B	206	ASP	2.4
1	A	332	GLU	2.3
1	C	413	ILE	2.3
1	D	437	ILE	2.3
1	A	377	VAL	2.3
1	B	291	VAL	2.3
1	D	206	ASP	2.3
1	A	413	ILE	2.3
1	A	359	LEU	2.3
1	D	200	VAL	2.3
1	A	363	ILE	2.3
1	C	362	ILE	2.3
1	C	414	ASP	2.3
1	D	203	ASN	2.3
1	B	190	LEU	2.2
1	D	338	HIS	2.2
1	B	269	PRO	2.2
1	D	188	PRO	2.2
1	A	362	ILE	2.2
1	A	372	ILE	2.2
1	B	357	GLU	2.2
1	C	436	ASN	2.2
1	B	362	ILE	2.2
1	B	213	GLY	2.2
1	B	216	PHE	2.2
1	C	319	PRO	2.2
1	A	287	GLN	2.2
1	B	192	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	201	LEU	2.2
1	A	314	ARG	2.2
1	A	218	GLU	2.2
1	B	314	ARG	2.2
1	B	388	LEU	2.1
1	A	338	HIS	2.1
1	A	325	ILE	2.1
1	D	202	LEU	2.1
1	D	217	ARG	2.1
1	C	285	SER	2.1
1	B	417	TRP	2.1
1	B	215	PRO	2.1
1	B	335	GLY	2.1
1	D	284	LEU	2.1
1	B	328	CYS	2.1
1	C	293	LYS	2.1
1	D	335	GLY	2.1
1	C	224	LEU	2.1
1	B	200	VAL	2.1
1	D	386	ASP	2.1
1	D	387	THR	2.1
1	C	365	ASP	2.0
1	D	226	ARG	2.0
1	C	198	LEU	2.0
1	C	191	THR	2.0
1	D	199	GLU	2.0
1	A	336	LYS	2.0
1	B	223	LEU	2.0
1	C	386	ASP	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 monosaccharides in this entry.

6.4 Ligands ⓘ

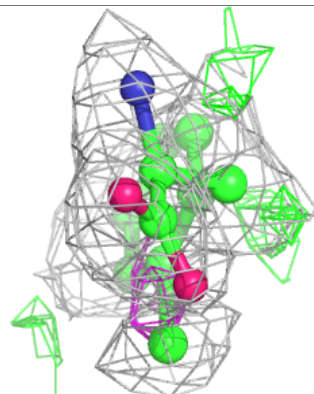
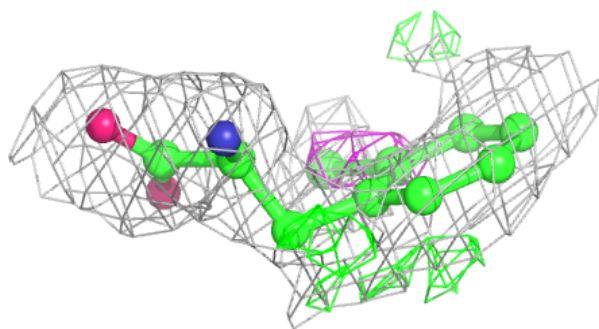
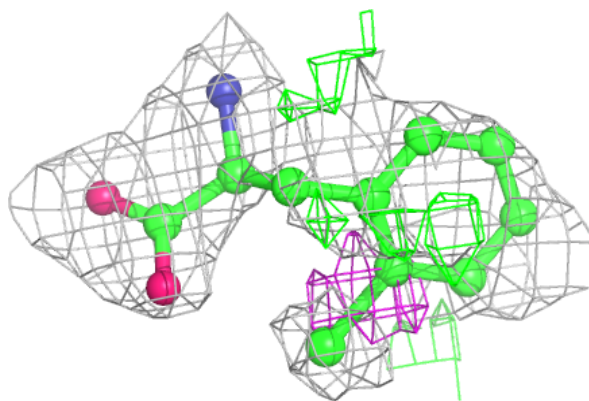
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	2L5	C	502	13/13	0.55	0.33	40,43,49,53	0
3	2L5	A	502	13/13	0.57	0.25	37,42,49,53	0
3	2L5	B	502	13/13	0.58	0.29	38,46,54,56	0
3	2L5	D	502	13/13	0.72	0.26	37,42,49,54	0
2	ANP	C	501	31/31	0.84	0.22	37,46,62,75	0
2	ANP	A	501	31/31	0.85	0.27	33,42,62,71	0
2	ANP	D	501	31/31	0.86	0.20	37,43,60,63	0
2	ANP	B	501	31/31	0.90	0.23	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.

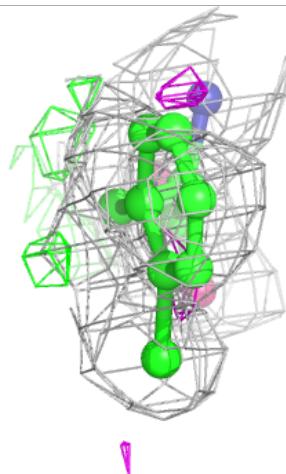
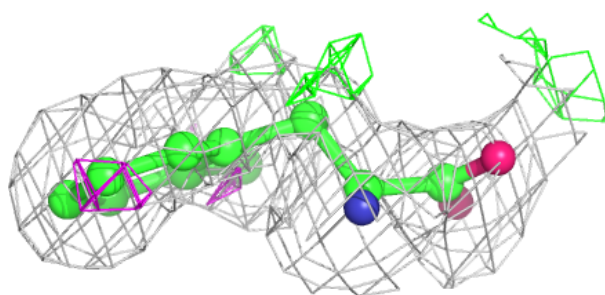
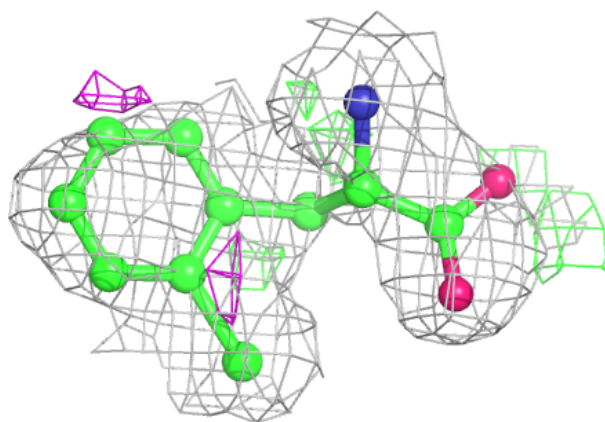
Electron density around 2L5 C 502:

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



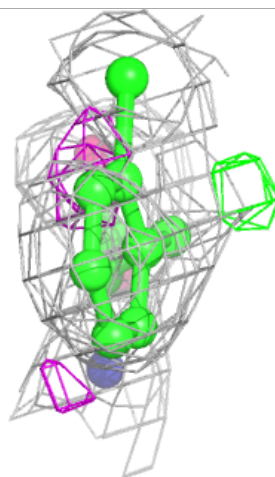
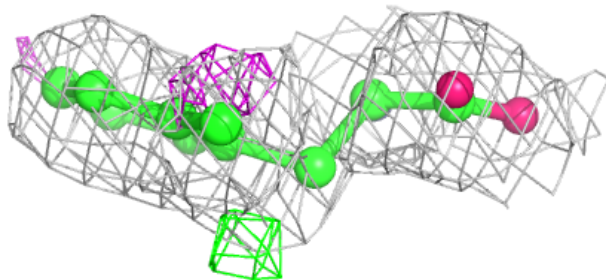
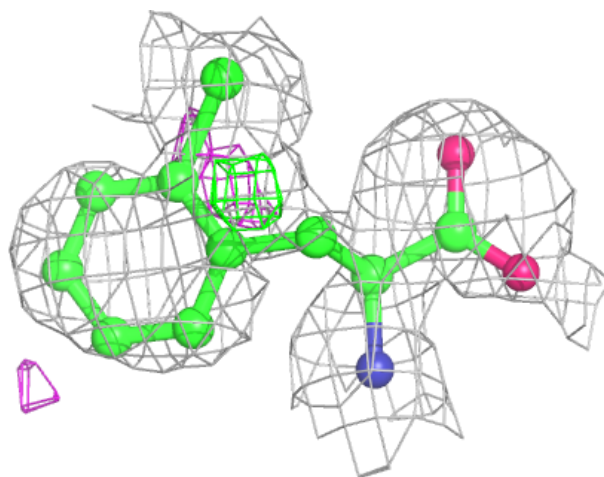
Electron density around 2L5 A 502:

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



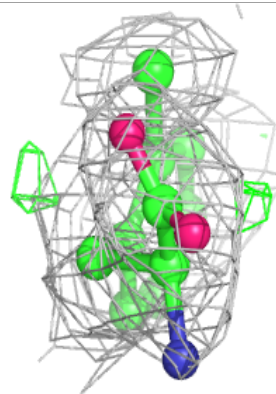
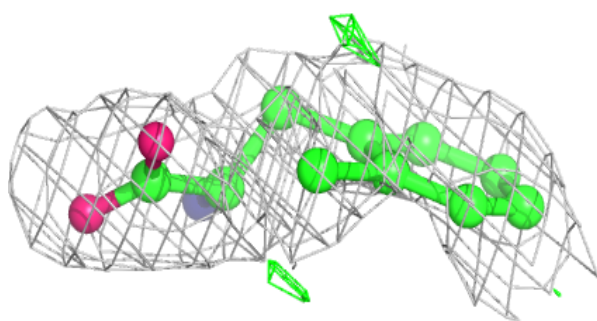
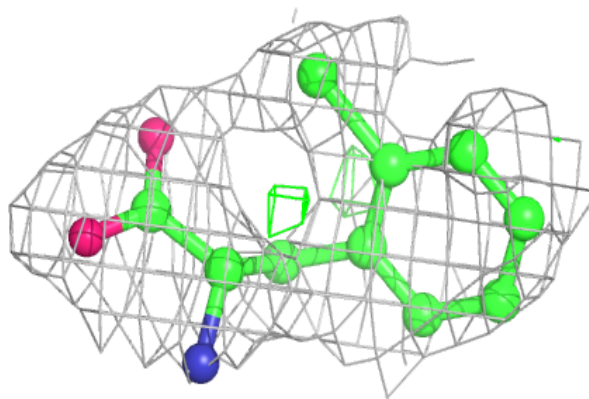
Electron density around 2L5 B 502:

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



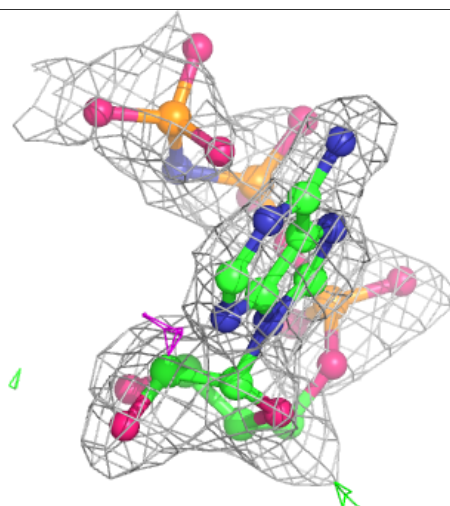
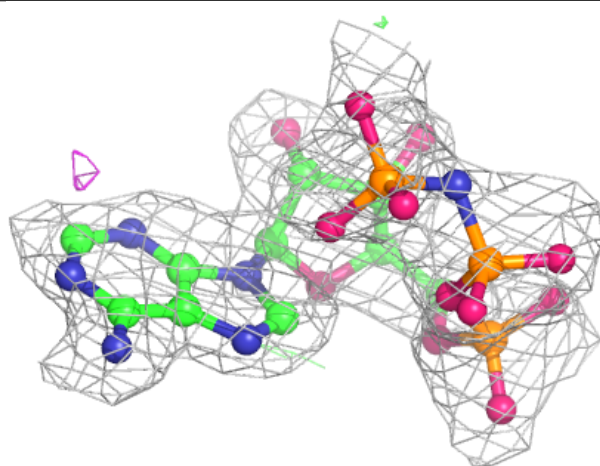
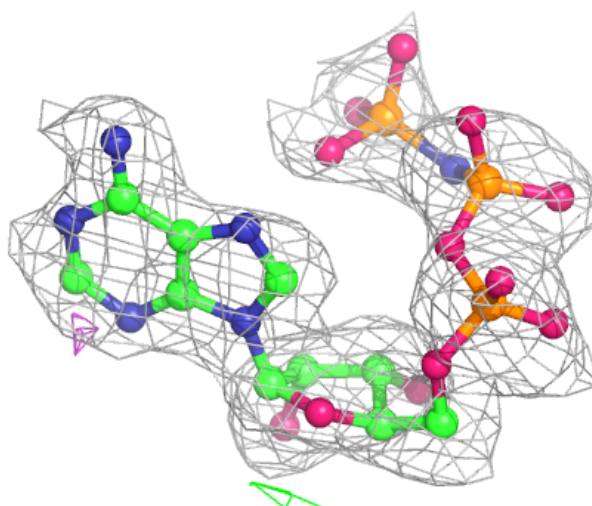
Electron density around 2L5 D 502:

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



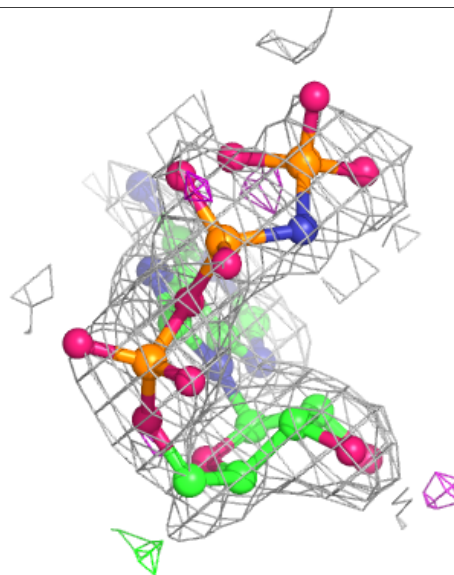
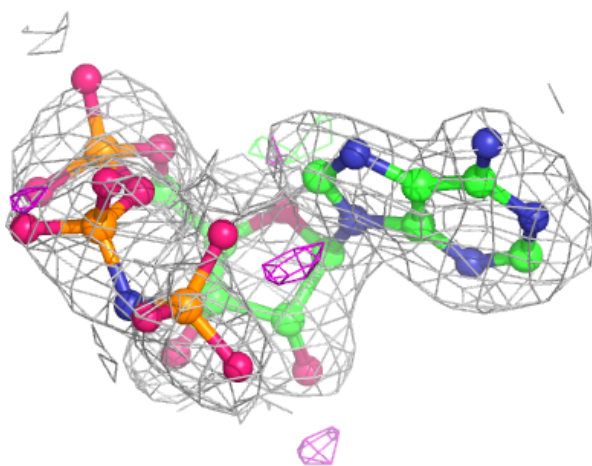
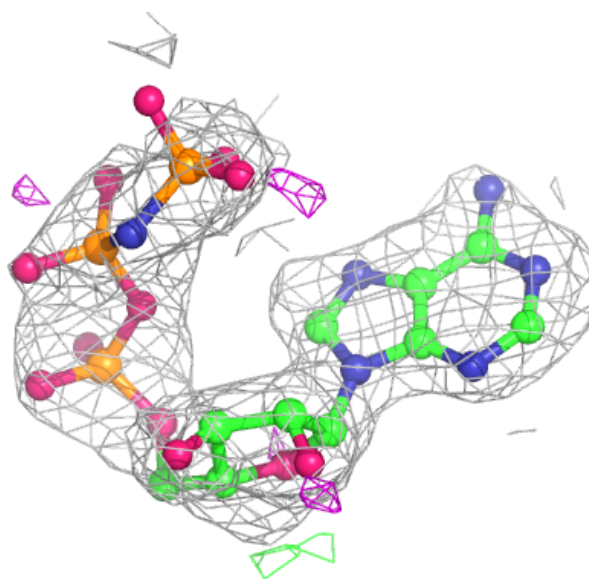
Electron density around ANP C 501:

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



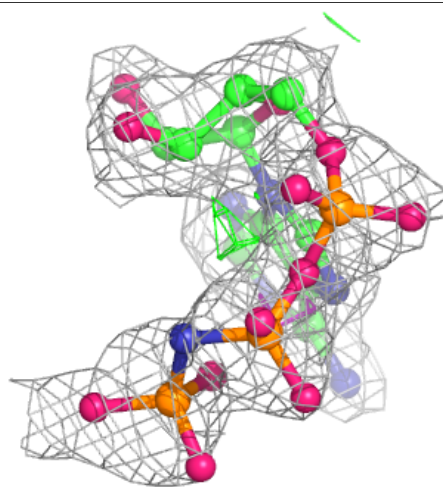
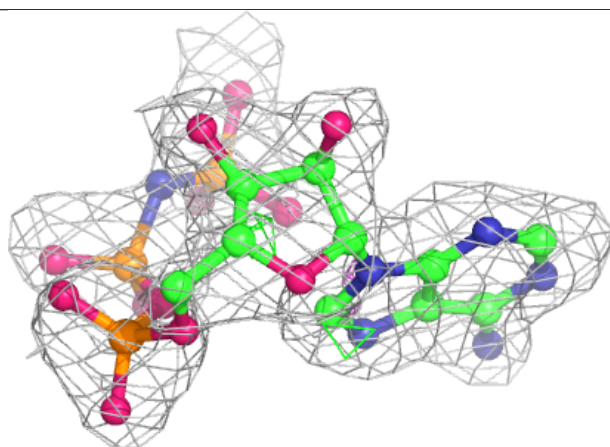
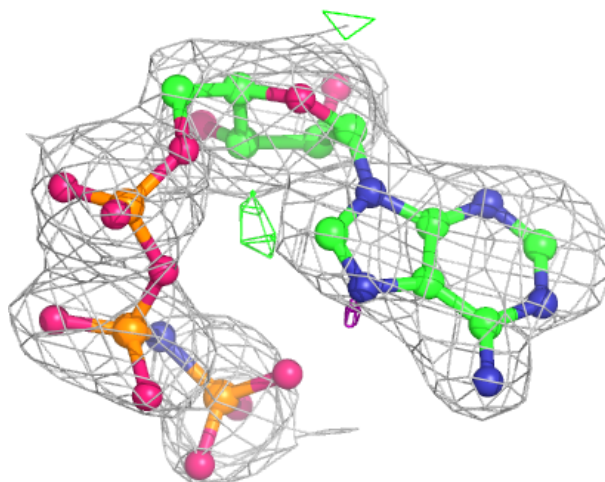
Electron density around ANP A 501:

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



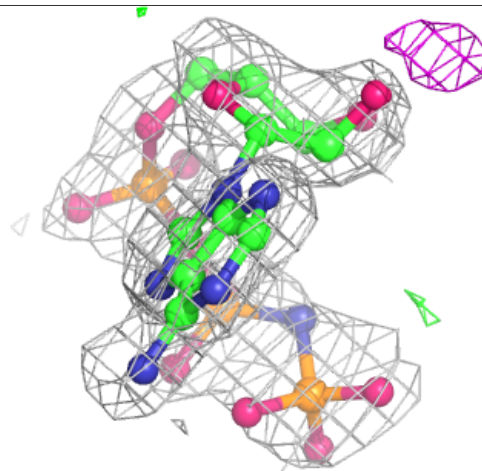
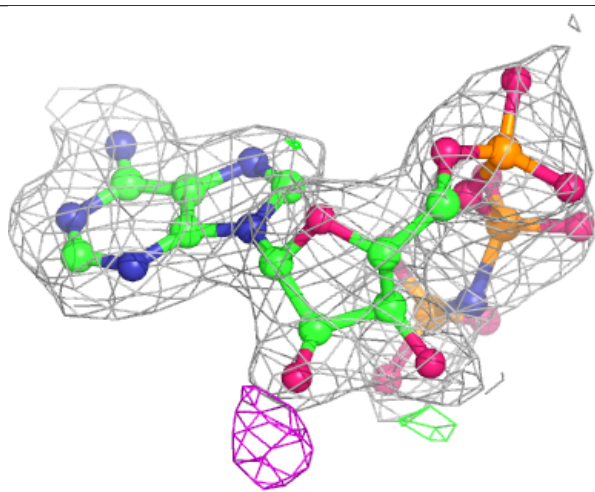
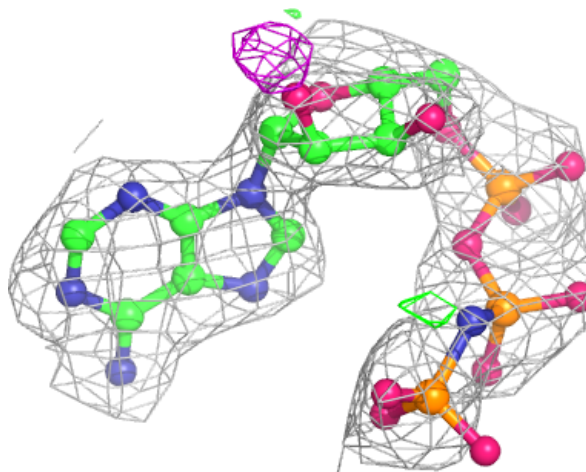
Electron density around ANP D 501:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.