



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:18 PM EDT

PDB ID : 5XIP / pdb_00005xip
Title : Crystal Structure of Eimeria tenella Prolyl-tRNA Synthetase (EtPRS) in complex with Halofuginone
Authors : Jain, V.; Manickam, Y.; Sharma, A.
Deposited on : 2017-04-26
Resolution : 3.10 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

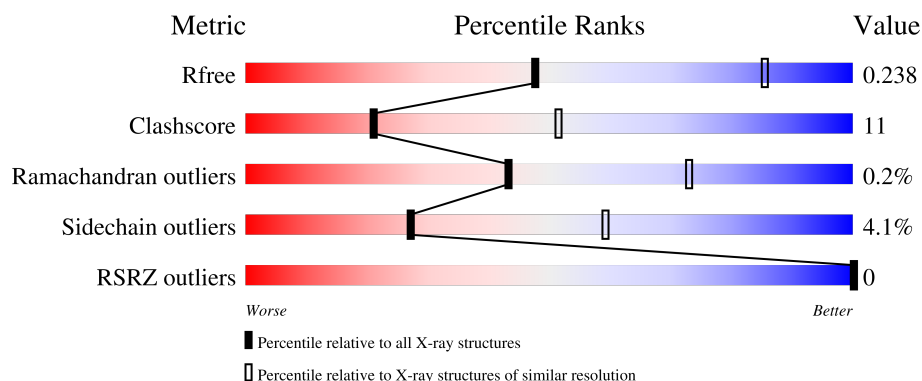
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	498	
1	B	498	
1	C	498	
1	D	498	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15058 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.

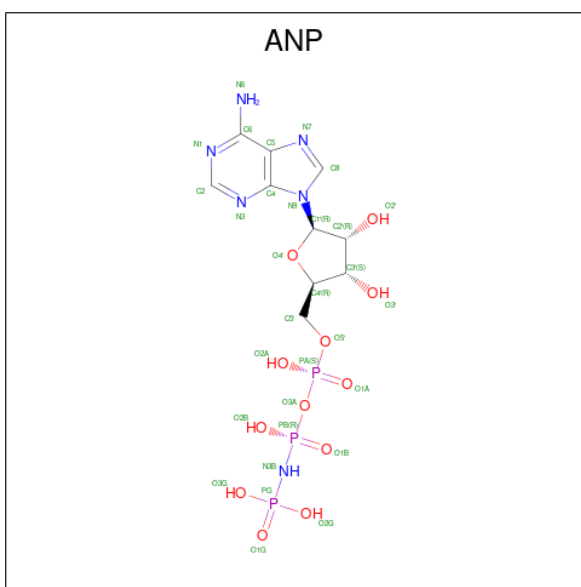
- Molecule 1 is a protein called Prolyl-tRNA synthetase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3767	2420	652	675	20			
1	B	475	Total	C	N	O	S	0	1	0
			3790	2430	653	688	19			
1	C	463	Total	C	N	O	S	0	1	0
			3633	2337	625	652	19			
1	D	457	Total	C	N	O	S	0	2	0
			3628	2334	622	652	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	250	GLY	-	expression tag	UNP U6KWI1
A	251	ALA	-	expression tag	UNP U6KWI1
A	252	MET	-	expression tag	UNP U6KWI1
B	250	GLY	-	expression tag	UNP U6KWI1
B	251	ALA	-	expression tag	UNP U6KWI1
B	252	MET	-	expression tag	UNP U6KWI1
C	250	GLY	-	expression tag	UNP U6KWI1
C	251	ALA	-	expression tag	UNP U6KWI1
C	252	MET	-	expression tag	UNP U6KWI1
D	250	GLY	-	expression tag	UNP U6KWI1
D	251	ALA	-	expression tag	UNP U6KWI1
D	252	MET	-	expression tag	UNP U6KWI1

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

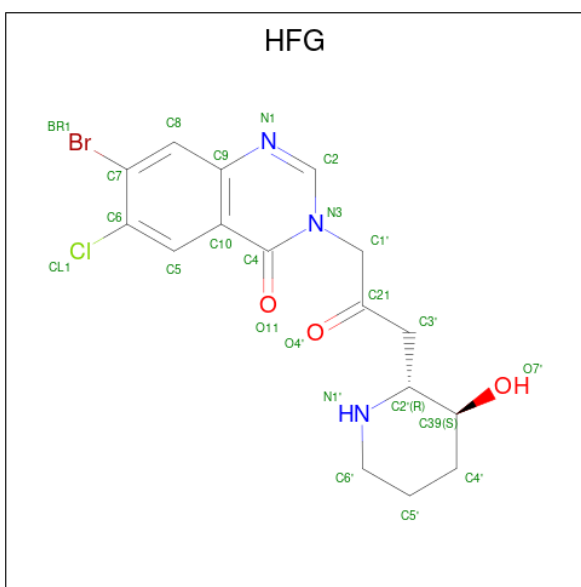


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is 7-bromo-6-chloro-3-{3-[(2R,3S)-3-hydroxypiperidin-2-yl]-2-oxopropyl}quinazolin-4(3H)-one (CCD ID: HFG) (formula: C₁₆H₁₇BrClN₃O₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
4	B	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
4	C	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		
4	D	1	Total	Br	C	Cl	N	O	0	0
			24	1	16	1	3	3		

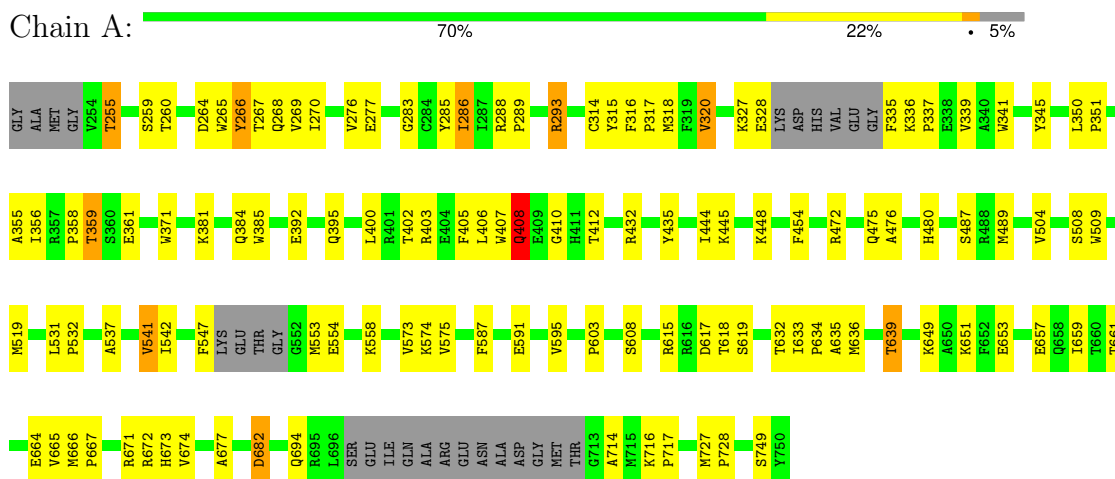
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	4	Total	O	0	0
			4	4		
5	B	4	Total	O	0	0
			4	4		
5	C	4	Total	O	0	0
			4	4		
5	D	4	Total	O	0	0
			4	4		

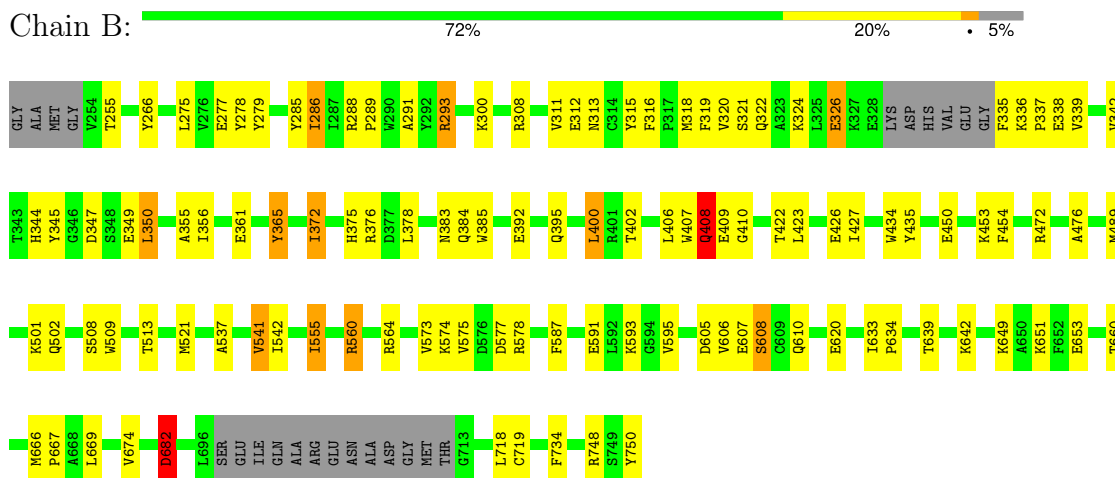
3 Residue-property plots

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: Prolyl-tRNA synthetase, putative

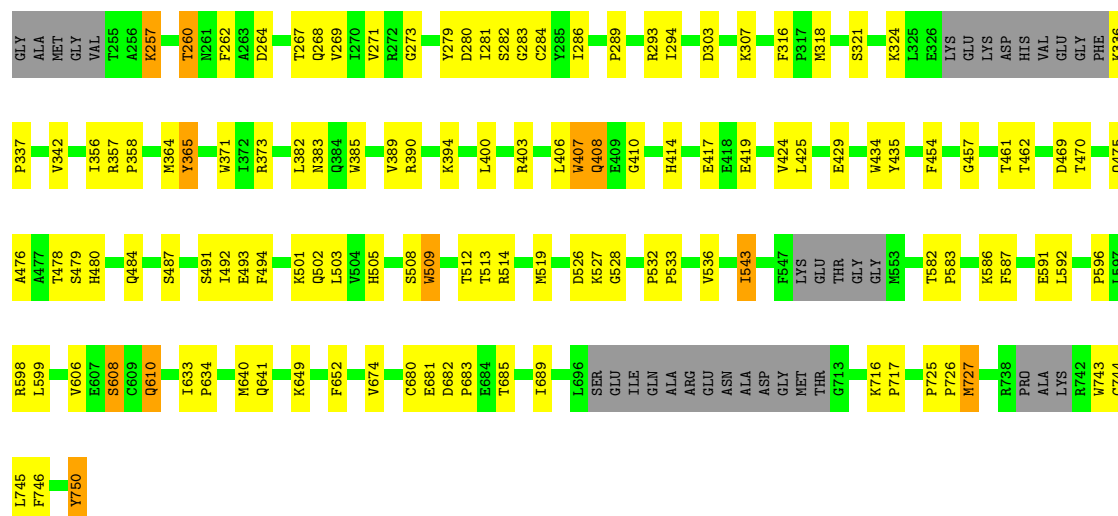


- Molecule 1: Prolyl-tRNA synthetase, putative



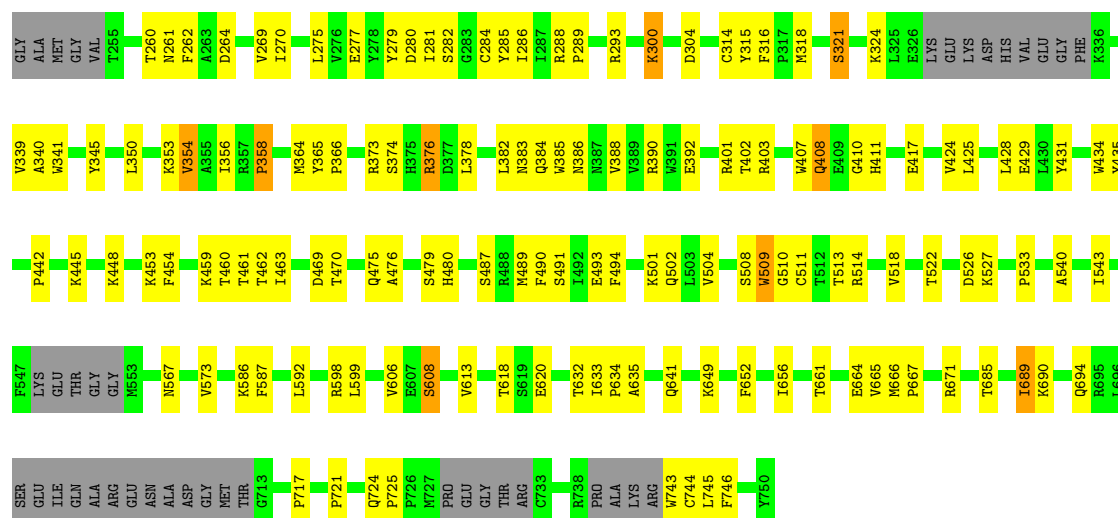
- Molecule 1: Prolyl-tRNA synthetase, putative





● Molecule 1: Prolyl-tRNA synthetase, putative

Chain D: 63% 27% 8%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	138.76Å 138.76Å 425.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.77 – 3.10 41.77 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.77-3.10) 95.6 (41.77-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.31 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.180 , 0.230 0.193 , 0.238	Depositor DCC
R_{free} test set	2003 reflections (3.78%)	wwPDB-VP
Wilson B-factor (Å ²)	63.6	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.459 for -h-k,k,-l	Xtriage
Reported twinning fraction	0.588 for H, K, L 0.412 for K, H, -L	Depositor
Outliers	0 of 53009 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15058	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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: HFG, ANP, MG

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	0.95	3/3865 (0.1%)	1.11	14/5248 (0.3%)
1	B	0.94	1/3890 (0.0%)	1.12	15/5283 (0.3%)
1	C	0.87	1/3727 (0.0%)	1.06	11/5065 (0.2%)
1	D	0.86	1/3726 (0.0%)	1.08	5/5062 (0.1%)
All	All	0.91	6/15208 (0.0%)	1.09	45/20658 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	TYR	CA-C	-5.48	1.45	1.52
1	C	365	TYR	C-O	-5.36	1.19	1.24
1	A	320	VAL	CA-C	5.35	1.58	1.52
1	A	267	THR	C-O	-5.26	1.18	1.24
1	B	365	TYR	C-O	-5.11	1.19	1.24
1	D	354	VAL	C-O	-5.02	1.19	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	608	SER	N-CA-C	-8.96	99.39	110.41
1	A	608	SER	N-CA-C	-8.70	99.71	110.41
1	D	608	SER	N-CA-C	-8.63	99.14	110.53
1	B	608	SER	N-CA-C	-8.11	100.44	110.41
1	D	665	VAL	N-CA-C	7.63	117.75	110.42
1	A	392	GLU	N-CA-C	7.52	121.72	109.76
1	D	470	THR	N-CA-C	7.43	119.38	111.28
1	B	326	GLU	N-CA-C	7.40	121.46	109.40
1	A	359	THR	N-CA-C	-6.83	99.31	108.74
1	B	408	GLN	N-CA-C	-6.39	99.49	109.72
1	A	608	SER	CA-C-N	-6.35	114.28	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	608	SER	C-N-CA	-6.35	114.28	122.79
1	B	395	GLN	N-CA-C	6.32	118.79	109.50
1	C	400	LEU	N-CA-C	6.22	118.86	111.33
1	C	469	ASP	N-CA-C	6.15	118.07	111.36
1	C	610	GLN	N-CA-C	6.15	116.20	108.45
1	C	543	ILE	CA-C-N	-6.05	113.74	119.85
1	C	543	ILE	C-N-CA	-6.05	113.74	119.85
1	C	727	MET	N-CA-C	6.02	119.41	110.32
1	A	408	GLN	N-CA-C	-5.89	100.29	109.72
1	A	682	ASP	CA-C-N	5.80	126.19	119.47
1	A	682	ASP	C-N-CA	5.80	126.19	119.47
1	A	260	THR	N-CA-C	5.74	120.30	112.04
1	B	308	ARG	N-CA-C	-5.63	105.14	111.28
1	A	339	VAL	N-CA-C	5.59	116.79	109.58
1	B	400	LEU	N-CA-C	5.53	116.99	111.07
1	B	392	GLU	N-CA-C	5.47	118.46	109.76
1	B	286	ILE	CB-CA-C	-5.40	105.46	111.35
1	C	389	VAL	N-CA-C	5.36	115.03	106.88
1	D	469	ASP	N-CA-C	5.32	117.16	111.36
1	A	286	ILE	CB-CA-C	-5.23	105.65	111.35
1	A	371	TRP	N-CA-C	5.21	116.96	111.28
1	C	492	ILE	CB-CA-C	5.21	118.43	111.19
1	C	470	THR	N-CA-C	5.14	117.79	111.82
1	B	278	TYR	CB-CA-C	5.14	118.83	109.83
1	A	395	GLN	N-CA-C	5.13	116.87	109.48
1	D	526	ASP	N-CA-C	5.13	119.16	113.01
1	B	682	ASP	CA-C-N	5.12	125.41	119.47
1	B	682	ASP	C-N-CA	5.12	125.41	119.47
1	B	311	VAL	N-CA-C	-5.11	102.50	109.55
1	B	286	ILE	N-CA-C	5.10	114.96	108.12
1	A	405	PHE	N-CA-C	5.08	116.96	108.99
1	B	350	LEU	N-CA-C	-5.06	103.31	110.29
1	B	734	PHE	N-CA-C	5.01	117.47	111.71
1	C	457	GLY	N-CA-C	5.01	119.90	111.04

There are no chirality outliers.

There are no planarity outliers.

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	3767	0	3694	74	0
1	B	3790	0	3698	74	0
1	C	3633	0	3524	86	0
1	D	3628	0	3514	105	0
2	A	31	0	13	2	0
2	B	31	0	13	0	0
2	C	31	0	13	2	0
2	D	31	0	13	4	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	24	0	17	6	0
4	B	24	0	17	7	0
4	C	24	0	17	6	0
4	D	24	0	17	4	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
All	All	15058	0	14550	325	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 11.

All (325) 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:407:TRP:CH2	4:B:1003:HFG:H8	1.92	1.04
1:A:407:TRP:CH2	4:A:1003:HFG:H8	2.01	0.95
1:A:356:ILE:HD11	1:B:356:ILE:HD11	1.56	0.88
1:A:407:TRP:CZ3	4:A:1003:HFG:H8	2.08	0.88
1:A:454:PHE:CE1	4:A:1003:HFG:H15	2.13	0.83
1:A:345:TYR:HD1	1:A:350:LEU:HD23	1.51	0.75
1:A:359:THR:OG1	1:A:361:GLU:OE1	2.03	0.75
1:D:279:TYR:HB3	1:D:284:CYS:O	1.86	0.74
1:D:390:ARG:NH1	2:D:1001:ANP:O2B	2.20	0.74
1:B:407:TRP:HH2	4:B:1003:HFG:H8	1.52	0.72
1:D:429:GLU:HA	1:D:429:GLU:OE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ARG:HD3	1:A:537:ALA:HA	1.73	0.71
1:A:435:TYR:CZ	1:A:476:ALA:HB1	2.25	0.71
1:D:435:TYR:CZ	1:D:476:ALA:HB1	2.25	0.71
1:B:454:PHE:CZ	4:B:1003:HFG:H1	2.26	0.70
1:D:378:LEU:HD11	1:D:504:VAL:HG12	1.73	0.70
1:D:725:PRO:HG2	1:D:743:TRP:CD1	2.26	0.70
1:A:318:MET:HE1	1:B:318:MET:SD	2.33	0.68
4:D:1003:HFG:O4'	4:D:1003:HFG:N1'	2.26	0.68
1:A:385:TRP:CZ3	1:A:408:GLN:HB2	2.28	0.68
1:C:487:SER:O	1:C:491:SER:N	2.26	0.68
1:C:414:HIS:HD1	1:C:419:GLU:HG2	1.59	0.67
1:D:480:HIS:NE2	4:D:1003:HFG:O7'	2.28	0.67
1:B:435:TYR:CZ	1:B:476:ALA:HB1	2.29	0.67
1:B:407:TRP:CZ3	4:B:1003:HFG:H8	2.30	0.67
1:A:435:TYR:CE2	1:A:476:ALA:HB1	2.29	0.66
1:A:318:MET:SD	1:B:318:MET:HE1	2.36	0.66
1:C:484:GLN:O	1:C:487:SER:HB2	1.96	0.66
1:A:649:LYS:O	1:A:653:GLU:HG2	1.95	0.66
1:B:372:ILE:HD13	1:B:378:LEU:HD21	1.77	0.65
1:B:339:VAL:HG22	4:B:1003:HFG:BR1	2.51	0.65
1:D:744:CYS:SG	1:D:745:LEU:N	2.70	0.65
1:B:320:VAL:HG12	1:B:355:ALA:HB3	1.79	0.65
1:C:407:TRP:CH2	4:C:1003:HFG:H8	2.31	0.65
1:D:618:THR:OG1	1:D:620:GLU:HG2	1.98	0.64
1:A:406:LEU:HD21	1:B:315:TYR:CE2	2.34	0.62
1:C:596:PRO:HB3	1:C:640:MET:SD	2.40	0.62
1:D:724:GLN:OE1	1:D:743:TRP:HB2	1.98	0.62
1:B:372:ILE:HD13	1:B:378:LEU:CD2	2.31	0.60
1:B:293:ARG:HH11	1:B:293:ARG:CG	2.14	0.60
1:A:283:GLY:HA3	1:A:403:ARG:HG3	1.85	0.59
1:D:285:TYR:HE1	1:D:402:THR:HG22	1.67	0.58
1:C:280:ASP:OD2	1:D:324:LYS:HD2	2.03	0.58
1:B:385:TRP:CZ3	1:B:408:GLN:HB2	2.39	0.58
1:C:316:PHE:CE1	1:C:364:MET:HE3	2.39	0.58
1:C:633:ILE:HB	1:C:634:PRO:HD3	1.84	0.58
1:B:682:ASP:OD1	1:B:682:ASP:C	2.47	0.58
1:B:422:THR:O	1:B:426:GLU:HG2	2.04	0.58
1:B:285:TYR:HE1	1:B:402:THR:HG22	1.69	0.57
1:C:744:CYS:SG	1:C:745:LEU:N	2.78	0.57
1:A:406:LEU:HD21	1:B:315:TYR:CZ	2.39	0.57
1:C:424:VAL:HG12	1:C:425:LEU:HD23	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:THR:O	1:A:619:SER:HB2	2.05	0.57
1:C:501:LYS:O	1:C:502:GLN:HG2	2.04	0.56
1:A:345:TYR:CD1	1:A:350:LEU:HD23	2.38	0.56
1:D:339:VAL:HG12	1:D:340:ALA:O	2.06	0.56
1:A:385:TRP:CE3	1:A:408:GLN:HB2	2.41	0.56
1:C:318:MET:SD	1:D:318:MET:HE1	2.46	0.56
1:D:649:LYS:O	1:D:652:PHE:HB3	2.05	0.56
1:B:277:GLU:HB3	1:B:286:ILE:HB	1.88	0.56
1:B:472:ARG:HH12	1:B:748:ARG:HB3	1.71	0.56
1:C:725:PRO:O	1:C:743:TRP:NE1	2.38	0.56
1:B:321:SER:OG	1:B:324:LYS:HB2	2.07	0.55
1:C:435:TYR:CZ	1:C:476:ALA:HB1	2.41	0.55
1:A:657:GLU:OE2	1:A:673:HIS:ND1	2.39	0.55
1:B:560:ARG:O	1:B:564:ARG:HG3	2.06	0.55
1:B:345:TYR:HD1	1:B:350:LEU:HD23	1.72	0.55
1:B:649:LYS:O	1:B:653:GLU:HG2	2.07	0.55
1:C:394:LYS:NZ	1:C:750:TYR:OXT	2.40	0.55
1:A:381:LYS:HA	1:A:412:THR:HG22	1.89	0.55
1:A:694:GLN:HB2	1:A:714:ALA:HB2	1.87	0.55
1:C:279:TYR:HB3	1:C:284:CYS:O	2.07	0.55
1:D:383:ASN:OD1	1:D:408:GLN:HG2	2.07	0.55
2:D:1001:ANP:O1A	4:D:1003:HFG:H2	2.08	0.55
1:A:487:SER:OG	1:A:504:VAL:HG23	2.06	0.54
1:C:480:HIS:NE2	4:C:1003:HFG:O7'	2.32	0.54
2:A:1001:ANP:O1A	4:A:1003:HFG:H17	2.07	0.54
1:C:407:TRP:HB3	1:C:512:THR:HG22	1.90	0.54
1:A:315:TYR:CZ	1:B:406:LEU:HD21	2.42	0.54
1:D:633:ILE:HB	1:D:634:PRO:HD3	1.89	0.54
1:B:407:TRP:CH2	4:B:1003:HFG:C5'	2.80	0.53
1:C:390:ARG:NH1	2:C:1001:ANP:O1A	2.40	0.53
1:B:587:PHE:O	1:B:591:GLU:HG3	2.09	0.53
1:C:371:TRP:NE1	1:D:277:GLU:OE2	2.40	0.53
1:C:286:ILE:HD13	1:D:316:PHE:CE2	2.44	0.53
1:D:316:PHE:CE1	1:D:364:MET:HG2	2.44	0.53
1:B:293:ARG:HH11	1:B:293:ARG:HG2	1.73	0.53
1:B:320:VAL:CG1	1:B:355:ALA:HB3	2.39	0.53
1:A:327:LYS:O	1:A:328:GLU:CB	2.56	0.53
1:B:336:LYS:N	1:B:337:PRO:CD	2.72	0.53
1:D:586:LYS:O	1:D:587:PHE:C	2.51	0.53
1:C:484:GLN:HG2	1:C:503:LEU:HB3	1.90	0.52
1:D:390:ARG:NH1	2:D:1001:ANP:O2A	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:MET:HE1	1:D:318:MET:SD	2.48	0.52
1:A:587:PHE:O	1:A:591:GLU:HG3	2.10	0.52
1:B:435:TYR:CE2	1:B:476:ALA:HB1	2.44	0.52
1:A:573:VAL:HG12	1:A:574:LYS:N	2.25	0.52
1:C:303:ASP:OD1	1:C:307:LYS:HD2	2.10	0.52
1:B:385:TRP:CE3	1:B:408:GLN:HB2	2.45	0.52
1:C:586:LYS:O	1:C:587:PHE:C	2.53	0.52
1:B:472:ARG:NH1	1:B:748:ARG:HB3	2.25	0.52
1:B:669:LEU:HB3	1:B:748:ARG:NH1	2.24	0.52
1:A:480:HIS:NE2	4:A:1003:HFG:O7'	2.31	0.52
1:D:533:PRO:HD2	1:D:641:GLN:OE1	2.10	0.51
1:D:513:THR:O	1:D:514:ARG:C	2.53	0.51
1:C:257:LYS:HA	1:C:526:ASP:OD1	2.11	0.51
1:C:342:VAL:HG11	1:D:340:ALA:HB1	1.93	0.51
1:D:685:THR:O	1:D:689:ILE:HG13	2.11	0.51
1:B:285:TYR:CE1	1:B:402:THR:HG22	2.46	0.51
1:D:598:ARG:C	1:D:599:LEU:HD12	2.37	0.50
1:B:345:TYR:CD1	1:B:350:LEU:HD23	2.47	0.50
1:A:264:ASP:O	1:A:268:GLN:HG3	2.11	0.50
1:D:354:VAL:O	1:D:354:VAL:HG23	2.12	0.50
1:D:434:TRP:C	1:D:434:TRP:CD1	2.89	0.50
1:D:667:PRO:O	1:D:671:ARG:HG3	2.11	0.50
1:A:407:TRP:CH2	4:A:1003:HFG:C5'	2.88	0.50
1:A:636:MET:O	1:A:639:THR:HB	2.12	0.50
1:A:682:ASP:C	1:A:682:ASP:OD1	2.55	0.50
1:C:267:THR:O	1:C:271:VAL:HG23	2.12	0.50
1:C:406:LEU:HD21	1:D:315:TYR:CE2	2.47	0.50
1:B:318:MET:HE2	1:B:356:ILE:HG23	1.94	0.49
1:B:409:GLU:O	1:B:409:GLU:HG3	2.12	0.49
1:B:606:VAL:O	1:B:608:SER:O	2.30	0.49
1:C:283:GLY:HA3	1:C:403:ARG:HG3	1.94	0.49
1:A:293:ARG:HH11	1:A:293:ARG:CG	2.25	0.49
1:B:573:VAL:HG22	1:B:574:LYS:H	1.78	0.49
1:D:321:SER:OG	1:D:324:LYS:HG3	2.12	0.49
1:B:669:LEU:HB3	1:B:748:ARG:HH12	1.76	0.49
1:C:417:GLU:HB2	1:C:505:HIS:ND1	2.27	0.49
1:C:475:GLN:NE2	1:C:478:THR:CG2	2.76	0.49
1:D:281:ILE:O	1:D:282:SER:C	2.55	0.49
1:C:324:LYS:HD2	1:D:280:ASP:OD2	2.12	0.49
1:D:401:ARG:NH2	2:D:1001:ANP:O3G	2.46	0.49
1:C:365:TYR:CD1	1:C:365:TYR:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:716:LYS:HG2	1:C:717:PRO:O	2.13	0.49
1:D:606:VAL:O	1:D:608:SER:O	2.31	0.49
1:C:454:PHE:CZ	4:C:1003:HFG:H1	2.48	0.48
1:D:364:MET:SD	1:D:411:HIS:CD2	3.06	0.48
1:A:293:ARG:HD3	1:A:537:ALA:CA	2.43	0.48
1:C:587:PHE:O	1:C:591:GLU:HG3	2.13	0.48
1:D:453:LYS:O	1:D:454:PHE:C	2.55	0.48
1:D:656:ILE:HD12	1:D:656:ILE:O	2.14	0.48
1:C:294:ILE:HD13	1:C:519:MET:HE1	1.96	0.48
1:B:375:HIS:NE2	1:B:376:ARG:HG3	2.29	0.48
1:C:373:ARG:O	1:C:494:PHE:HA	2.14	0.48
1:C:434:TRP:CD1	1:C:434:TRP:C	2.91	0.48
1:D:341:TRP:CE3	1:D:353:LYS:HD2	2.49	0.48
1:A:432:ARG:HD3	1:A:445:LYS:HE3	1.94	0.48
1:C:606:VAL:O	1:C:608:SER:O	2.31	0.48
1:D:410:GLY:O	1:D:508:SER:HA	2.12	0.48
1:D:721:PRO:O	1:D:724:GLN:HG2	2.13	0.48
1:D:300:LYS:HE3	1:D:304:ASP:OD2	2.13	0.48
1:C:414:HIS:ND1	1:C:419:GLU:HG2	2.26	0.47
1:D:606:VAL:C	1:D:608:SER:O	2.57	0.47
2:C:1001:ANP:O2B	4:C:1003:HFG:H17	2.14	0.47
1:D:493:GLU:HA	1:D:502:GLN:O	2.13	0.47
1:A:265:TRP:O	1:A:268:GLN:HB2	2.14	0.47
1:A:716:LYS:HB2	1:A:717:PRO:HD2	1.96	0.47
1:A:336:LYS:N	1:A:337:PRO:HD2	2.29	0.47
1:C:587:PHE:CD1	1:C:598:ARG:HD2	2.50	0.47
1:D:479:SER:HA	1:D:509:TRP:HB3	1.95	0.47
1:A:410:GLY:O	1:A:508:SER:HA	2.15	0.47
1:B:542:ILE:HB	1:B:575:VAL:HG22	1.95	0.47
1:A:266:TYR:HA	1:A:269:VAL:HG22	1.96	0.47
1:D:489:MET:HE2	1:D:489:MET:HB3	1.82	0.47
1:D:300:LYS:O	1:D:300:LYS:HG3	2.14	0.47
1:A:255:THR:H	1:A:268:GLN:HE22	1.62	0.46
1:A:615:ARG:NH2	1:A:617:ASP:OD2	2.48	0.46
1:C:461:THR:OG1	1:C:479:SER:O	2.33	0.46
1:C:533:PRO:HD2	1:C:641:GLN:OE1	2.16	0.46
1:D:424:VAL:HG12	1:D:425:LEU:HD23	1.97	0.46
1:B:555:ILE:HG13	1:B:606:VAL:HG21	1.97	0.46
1:A:487:SER:OG	1:A:504:VAL:CG2	2.63	0.46
1:B:633:ILE:HB	1:B:634:PRO:HD3	1.97	0.46
1:D:487:SER:O	1:D:491:SER:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:599:LEU:HG	1:D:613:VAL:HG22	1.97	0.46
1:D:279:TYR:CB	1:D:284:CYS:O	2.59	0.46
1:D:725:PRO:HG2	1:D:743:TRP:CG	2.50	0.46
1:B:322:GLN:NE2	1:B:326:GLU:OE2	2.47	0.46
1:A:633:ILE:HB	1:A:634:PRO:HD3	1.97	0.46
1:C:479:SER:HA	1:C:509:TRP:HB3	1.97	0.46
1:A:727:MET:O	1:A:728:PRO:C	2.58	0.46
1:C:383:ASN:OD1	1:C:408:GLN:HG2	2.16	0.46
1:B:365:TYR:CD1	1:B:365:TYR:N	2.82	0.46
1:D:365:TYR:CD1	1:D:365:TYR:N	2.83	0.46
1:C:336:LYS:N	1:C:337:PRO:CD	2.78	0.46
1:D:518:VAL:O	1:D:522:THR:OG1	2.28	0.46
1:B:293:ARG:CG	1:B:293:ARG:NH1	2.73	0.45
1:B:316:PHE:HB2	1:B:384:GLN:HE22	1.81	0.45
1:B:660:THR:O	1:B:660:THR:HG22	2.15	0.45
1:D:261:ASN:OD1	1:D:264:ASP:HB2	2.16	0.45
1:D:527:LYS:O	1:D:592:LEU:HD23	2.16	0.45
1:D:543:ILE:HD12	1:D:598:ARG:CD	2.46	0.45
1:A:320:VAL:CG1	1:A:355:ALA:HB3	2.47	0.45
1:C:289:PRO:HG3	1:D:382:LEU:HD22	1.99	0.45
1:D:431:TYR:CE1	1:D:511:CYS:HB2	2.51	0.45
1:A:336:LYS:HE2	1:B:347:ASP:OD1	2.17	0.45
1:A:542:ILE:HB	1:A:575:VAL:HG22	1.98	0.45
1:C:725:PRO:HA	1:C:726:PRO:HD3	1.85	0.45
1:C:356:ILE:HD11	1:D:356:ILE:HD11	1.99	0.45
1:A:554:GLU:O	1:A:558:LYS:HG2	2.17	0.45
1:A:316:PHE:HB2	1:A:384:GLN:HE22	1.82	0.44
1:D:318:MET:HE2	1:D:356:ILE:HG23	1.99	0.44
1:D:392:GLU:O	1:D:403:ARG:NH2	2.50	0.44
1:C:462:THR:OG1	1:C:475:GLN:HG3	2.17	0.44
1:D:385:TRP:CE3	1:D:408:GLN:HB2	2.52	0.44
1:A:541:VAL:HG12	1:A:595:VAL:HG11	2.00	0.44
1:C:269:VAL:O	1:C:273:GLY:N	2.51	0.44
1:B:275:LEU:HD22	1:B:291:ALA:HB2	2.00	0.44
1:D:345:TYR:O	1:D:345:TYR:CD2	2.70	0.44
1:A:661:THR:HG22	1:A:664:GLU:OE1	2.17	0.44
1:C:633:ILE:O	1:C:634:PRO:C	2.60	0.44
1:C:717:PRO:HB3	1:C:746:PHE:CE2	2.52	0.44
1:B:293:ARG:HD3	1:B:537:ALA:HA	1.99	0.44
1:C:262:PHE:CD1	1:C:262:PHE:C	2.96	0.44
1:C:608:SER:HB2	1:C:610:GLN:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:428:LEU:HD23	1:D:445:LYS:HG2	1.99	0.44
1:A:666:MET:N	1:A:667:PRO:HD2	2.32	0.44
1:C:269:VAL:HG12	1:C:528:GLY:HA2	2.00	0.44
1:C:527:LYS:HD2	1:C:591:GLU:HB3	2.00	0.44
1:D:262:PHE:CD1	1:D:262:PHE:C	2.95	0.44
1:C:685:THR:O	1:C:689:ILE:HG13	2.17	0.43
1:D:345:TYR:CD1	1:D:350:LEU:HD23	2.53	0.43
1:A:472:ARG:NH1	1:A:749:SER:O	2.49	0.43
1:C:281:ILE:O	1:C:282:SER:C	2.60	0.43
4:C:1003:HFG:O4'	4:C:1003:HFG:N1'	2.51	0.43
1:D:285:TYR:CE1	1:D:402:THR:HG22	2.50	0.43
1:B:577:ASP:O	1:B:578:ARG:C	2.60	0.43
1:D:666:MET:N	1:D:667:PRO:CD	2.81	0.43
1:C:268:GLN:O	1:C:269:VAL:C	2.61	0.43
1:C:527:LYS:O	1:C:592:LEU:HD23	2.18	0.43
1:C:543:ILE:HD12	1:C:598:ARG:HD2	2.00	0.43
4:B:1003:HFG:O4'	4:B:1003:HFG:N1'	2.51	0.43
1:D:314:CYS:O	1:D:384:GLN:HB3	2.18	0.43
1:A:277:GLU:HB3	1:A:286:ILE:HB	2.01	0.43
1:A:448:LYS:HE2	1:A:475:GLN:OE1	2.18	0.43
1:A:671:ARG:O	1:A:672:ARG:HB2	2.18	0.43
1:B:450:GLU:O	1:B:453:LYS:HG2	2.18	0.43
1:D:725:PRO:HG2	1:D:743:TRP:NE1	2.33	0.43
1:B:607:GLU:C	1:B:608:SER:O	2.58	0.43
1:C:598:ARG:C	1:C:599:LEU:HD12	2.44	0.43
1:C:649:LYS:O	1:C:652:PHE:HB3	2.19	0.43
1:B:605:ASP:HB3	1:B:610:GLN:O	2.18	0.43
1:C:382:LEU:HD22	1:D:289:PRO:HG3	2.00	0.43
1:D:374:SER:CB	1:D:376[A]:ARG:HG3	2.48	0.43
1:D:374:SER:OG	1:D:376[A]:ARG:HG3	2.18	0.43
1:D:540:ALA:HB3	1:D:573:VAL:HG12	2.01	0.43
1:D:408:GLN:HE22	1:D:510:GLY:HA2	1.82	0.42
1:B:606:VAL:C	1:B:608:SER:O	2.62	0.42
1:C:318:MET:HE2	1:C:356:ILE:HG23	2.01	0.42
1:D:374:SER:HB3	1:D:376[A]:ARG:HG3	2.01	0.42
1:A:547:PHE:CE2	1:A:603:PRO:HG2	2.54	0.42
1:D:366:PRO:HD3	1:D:490:PHE:CD2	2.55	0.42
1:D:462:THR:OG1	1:D:475:GLN:HG3	2.19	0.42
1:C:429:GLU:OE1	1:C:429:GLU:HA	2.19	0.42
1:C:543:ILE:HD12	1:C:598:ARG:CD	2.50	0.42
1:D:407:TRP:CH2	4:D:1003:HFG:H8	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:ARG:CG	1:A:293:ARG:NH1	2.82	0.42
1:A:315:TYR:CE2	1:B:406:LEU:HD21	2.55	0.42
1:A:553:MET:HA	1:A:553:MET:HE2	2.02	0.42
1:D:429:GLU:OE1	1:D:429:GLU:CA	2.56	0.42
1:A:341:TRP:CZ3	1:A:355:ALA:HB2	2.55	0.42
1:B:541:VAL:HG12	1:B:595:VAL:HG11	2.02	0.42
1:D:487:SER:O	1:D:491:SER:HA	2.20	0.42
1:C:407:TRP:CZ3	4:C:1003:HFG:H8	2.55	0.42
1:A:350:LEU:O	1:A:351:PRO:C	2.61	0.42
1:B:319:PHE:CE1	1:B:342:VAL:HG21	2.55	0.42
1:C:316:PHE:CE2	1:D:286:ILE:HD13	2.55	0.42
1:C:493:GLU:HA	1:C:502:GLN:O	2.18	0.42
1:D:661:THR:O	1:D:664:GLU:OE1	2.38	0.42
1:A:293:ARG:HH11	1:A:293:ARG:HG2	1.85	0.42
1:D:358:PRO:HA	1:D:388:VAL:HG13	2.01	0.42
1:B:313:ASN:HA	1:B:383:ASN:O	2.20	0.42
1:A:288:ARG:HB3	1:A:289:PRO:HD2	2.02	0.41
1:A:659:ILE:CD1	1:A:665:VAL:HG22	2.50	0.41
1:D:269:VAL:HG23	1:D:270:ILE:HG23	2.02	0.41
1:C:513:THR:O	1:C:514:ARG:C	2.62	0.41
1:C:532:PRO:HA	1:C:533:PRO:HD3	1.86	0.41
1:D:345:TYR:O	1:D:345:TYR:CG	2.71	0.41
1:A:444:ILE:HG22	1:A:445:LYS:O	2.21	0.41
1:B:666:MET:N	1:B:667:PRO:CD	2.83	0.41
1:B:718:LEU:O	1:B:719:CYS:HB3	2.20	0.41
1:C:680:CYS:O	1:C:681:GLU:CB	2.68	0.41
1:A:659:ILE:CG1	1:A:677:ALA:HB2	2.51	0.41
1:D:448:LYS:HE2	1:D:475:GLN:HE21	1.84	0.41
1:A:285:TYR:HE1	1:A:402:THR:HG22	1.85	0.41
1:A:314:CYS:O	1:A:384:GLN:HB3	2.21	0.41
1:B:266:TYR:CE1	1:B:521:MET:HE3	2.55	0.41
1:D:356:ILE:O	1:D:358:PRO:HD3	2.20	0.41
1:B:288:ARG:O	1:B:289:PRO:C	2.63	0.41
1:B:423:LEU:HD23	1:B:427:ILE:HG12	2.02	0.41
1:B:434:TRP:CD1	1:B:434:TRP:C	2.99	0.41
1:C:410:GLY:O	1:C:508:SER:HA	2.20	0.41
1:D:275:LEU:O	1:D:288:ARG:HG3	2.21	0.41
1:D:373:ARG:HA	1:D:373:ARG:HD3	1.90	0.41
1:D:459:LYS:HG2	1:D:460:THR:N	2.36	0.41
1:D:632:THR:O	1:D:635:ALA:HB3	2.20	0.41
1:C:533:PRO:HA	1:C:536:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:448:LYS:CE	1:D:475:GLN:NE2	2.84	0.41
1:B:318:MET:HE3	1:B:318:MET:HB2	1.90	0.41
1:B:410:GLY:O	1:B:508:SER:HA	2.21	0.41
1:B:501:LYS:O	1:B:502:GLN:HG2	2.21	0.41
1:C:257:LYS:HB2	1:C:260:THR:HB	2.01	0.41
1:C:385:TRP:CE3	1:C:408:GLN:HB2	2.55	0.41
1:C:407:TRP:CD1	1:C:407:TRP:C	2.99	0.41
1:C:682:ASP:HA	1:C:683:PRO:HD2	1.98	0.41
1:D:448:LYS:HE2	1:D:475:GLN:NE2	2.35	0.41
1:D:461:THR:OG1	1:D:479:SER:O	2.37	0.41
1:D:717:PRO:HB3	1:D:746:PHE:CE2	2.55	0.41
1:A:519:MET:HE3	1:A:519:MET:HB3	2.00	0.41
1:C:493:GLU:HG3	1:C:503:LEU:HD23	2.04	0.41
1:D:442:PRO:HG3	1:D:649:LYS:HA	2.02	0.41
1:C:264:ASP:O	1:C:268:GLN:HG3	2.21	0.40
1:D:373:ARG:O	1:D:494:PHE:HA	2.21	0.40
1:A:531:LEU:HA	1:A:532:PRO:HD3	1.91	0.40
1:A:632:THR:O	1:A:635:ALA:HB3	2.21	0.40
1:D:280:ASP:OD1	1:D:281:ILE:HG13	2.21	0.40
1:C:508:SER:C	1:C:509:TRP:CD1	2.99	0.40
1:D:386:ASN:OD1	1:D:407:TRP:NE1	2.54	0.40
1:D:487:SER:O	1:D:491:SER:CA	2.69	0.40
1:D:690:LYS:O	1:D:694:GLN:CB	2.69	0.40
2:A:1001:ANP:H8	2:A:1001:ANP:H3'	2.04	0.40
1:C:582:THR:HA	1:C:583:PRO:HD3	2.00	0.40
1:A:317:PRO:HG2	1:B:279:TYR:CE2	2.57	0.40
1:B:344:HIS:HD2	1:B:347:ASP:O	2.04	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	463/498 (93%)	431 (93%)	31 (7%)	1 (0%)	43	73
1	B	470/498 (94%)	433 (92%)	37 (8%)	0	100	100
1	C	454/498 (91%)	417 (92%)	36 (8%)	1 (0%)	43	73
1	D	447/498 (90%)	407 (91%)	39 (9%)	1 (0%)	43	73
All	All	1834/1992 (92%)	1688 (92%)	143 (8%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	PRO
1	C	358	PRO
1	D	358	PRO

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	393/429 (92%)	379 (96%)	14 (4%)	31	62
1	B	394/429 (92%)	369 (94%)	25 (6%)	16	45
1	C	369/429 (86%)	358 (97%)	11 (3%)	36	65
1	D	373/429 (87%)	360 (96%)	13 (4%)	32	62
All	All	1529/1716 (89%)	1466 (96%)	63 (4%)	27	59

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	255	THR
1	A	259	SER
1	A	270	ILE
1	A	276	VAL
1	A	293	ARG
1	A	335	PHE
1	A	400	LEU
1	A	408	GLN

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Mol	Chain	Res	Type
1	A	489	MET
1	A	509	TRP
1	A	541	VAL
1	A	639	THR
1	A	651	LYS
1	A	674	VAL
1	B	255	THR
1	B	293	ARG
1	B	300	LYS
1	B	312	GLU
1	B	335	PHE
1	B	338	GLU
1	B	349	GLU
1	B	361	GLU
1	B	372	ILE
1	B	400	LEU
1	B	408	GLN
1	B	489	MET
1	B	509	TRP
1	B	513	THR
1	B	541	VAL
1	B	555	ILE
1	B	560	ARG
1	B	593	LYS
1	B	620	GLU
1	B	639	THR
1	B	642	LYS
1	B	651	LYS
1	B	674	VAL
1	B	682	ASP
1	B	750	TYR
1	C	257	LYS
1	C	260	THR
1	C	293	ARG
1	C	321	SER
1	C	357	ARG
1	C	407	TRP
1	C	408	GLN
1	C	509	TRP
1	C	674	VAL
1	C	727	MET
1	C	750	TYR

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Mol	Chain	Res	Type
1	D	260	THR
1	D	293	ARG
1	D	300	LYS
1	D	321	SER
1	D	376[A]	ARG
1	D	376[B]	ARG
1	D	408	GLN
1	D	417	GLU
1	D	463	ILE
1	D	501	LYS
1	D	509	TRP
1	D	567	ASN
1	D	689	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN
1	A	475	GLN
1	A	588	ASN
1	C	299	GLN
1	C	475	GLN
1	C	506	GLN
1	C	588	ASN
1	C	610	GLN
1	D	408	GLN
1	D	505	HIS
1	D	506	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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
4	HFG	A	1003	-	26,26,26	0.69	0	29,37,37	0.82	0
2	ANP	D	1001	3	33,33,33	1.66	3 (9%)	45,52,52	1.43	8 (17%)
4	HFG	B	1003	-	26,26,26	0.68	0	29,37,37	0.82	0
2	ANP	C	1001	3	33,33,33	2.13	7 (21%)	45,52,52	1.32	6 (13%)
2	ANP	A	1001	3	33,33,33	1.45	2 (6%)	45,52,52	0.85	2 (4%)
4	HFG	C	1003	-	26,26,26	0.69	0	29,37,37	0.82	0
4	HFG	D	1003	-	26,26,26	0.87	0	29,37,37	0.83	0
2	ANP	B	1001	3	33,33,33	1.51	2 (6%)	45,52,52	1.01	3 (6%)

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
4	HFG	A	1003	-	-	0/8/19/19	0/3/3/3
2	ANP	D	1001	3	-	5/18/38/38	0/3/3/3
4	HFG	B	1003	-	-	0/8/19/19	0/3/3/3
2	ANP	C	1001	3	-	3/18/38/38	0/3/3/3
2	ANP	A	1001	3	-	5/18/38/38	0/3/3/3
4	HFG	C	1003	-	-	0/8/19/19	0/3/3/3
4	HFG	D	1003	-	-	2/8/19/19	0/3/3/3
2	ANP	B	1001	3	-	6/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ANP	PG-O1G	6.72	1.56	1.46
2	B	1001	ANP	PG-O1G	6.68	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ANP	PG-O1G	6.16	1.55	1.46
2	C	1001	ANP	PB-O2B	-5.79	1.41	1.56
2	A	1001	ANP	PB-O1B	5.15	1.54	1.46
2	A	1001	ANP	PB-O2B	-4.87	1.43	1.56
2	C	1001	ANP	PG-O3G	-4.50	1.44	1.56
2	C	1001	ANP	PB-O1B	4.46	1.52	1.46
2	D	1001	ANP	PG-O3G	-3.93	1.46	1.56
2	B	1001	ANP	PG-O3G	-3.92	1.46	1.56
2	C	1001	ANP	PG-N3B	3.51	1.72	1.63
2	D	1001	ANP	PG-N3B	2.75	1.70	1.63
2	C	1001	ANP	PB-N3B	2.64	1.70	1.63
2	C	1001	ANP	PB-O3A	2.02	1.61	1.59

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1001	ANP	C4-C5-N7	-3.64	106.42	110.58
2	D	1001	ANP	C5-C4-N3	-3.47	121.94	126.72
2	D	1001	ANP	C5-C4-N9	3.35	109.46	105.81
2	D	1001	ANP	O2G-PG-O1G	-3.13	105.60	113.45
2	B	1001	ANP	O2G-PG-O1G	-3.12	105.62	113.45
2	C	1001	ANP	C6-C5-N7	2.92	137.72	132.09
2	C	1001	ANP	O2G-PG-O1G	-2.88	106.24	113.45
2	C	1001	ANP	O1G-PG-N3B	-2.87	107.55	111.77
2	A	1001	ANP	O1G-PG-N3B	-2.58	107.97	111.77
2	C	1001	ANP	C5-C4-N9	2.47	108.50	105.81
2	D	1001	ANP	C6-C5-N7	2.27	136.47	132.09
2	D	1001	ANP	C5-N7-C8	2.25	106.99	103.45
2	C	1001	ANP	C6-C5-C4	-2.25	114.10	117.18
2	B	1001	ANP	C5-C4-N3	-2.25	123.62	126.72
2	D	1001	ANP	O1B-PB-N3B	2.24	115.07	111.77
2	C	1001	ANP	C4-C5-N7	-2.14	108.14	110.58
2	A	1001	ANP	O1B-PB-N3B	2.07	114.83	111.77
2	B	1001	ANP	O1B-PB-N3B	2.07	114.81	111.77
2	D	1001	ANP	C2-N3-C4	2.05	116.85	111.83

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ANP	PB-N3B-PG-O1G
2	A	1001	ANP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
2	A	1001	ANP	C5'-O5'-PA-O2A
2	A	1001	ANP	C5'-O5'-PA-O3A
2	B	1001	ANP	PB-N3B-PG-O1G
2	B	1001	ANP	PG-N3B-PB-O1B
2	B	1001	ANP	PA-O3A-PB-O2B
2	B	1001	ANP	C5'-O5'-PA-O2A
2	B	1001	ANP	C5'-O5'-PA-O3A
2	C	1001	ANP	C5'-O5'-PA-O1A
2	C	1001	ANP	C5'-O5'-PA-O2A
2	C	1001	ANP	C5'-O5'-PA-O3A
2	D	1001	ANP	PB-N3B-PG-O1G
2	D	1001	ANP	PG-N3B-PB-O1B
2	D	1001	ANP	C5'-O5'-PA-O1A
2	D	1001	ANP	C5'-O5'-PA-O2A
2	D	1001	ANP	C5'-O5'-PA-O3A
4	D	1003	HFG	N1'-C2'-C3'-C21
4	D	1003	HFG	C39-C2'-C3'-C21
2	A	1001	ANP	PB-O3A-PA-O2A
2	B	1001	ANP	PA-O3A-PB-O1B

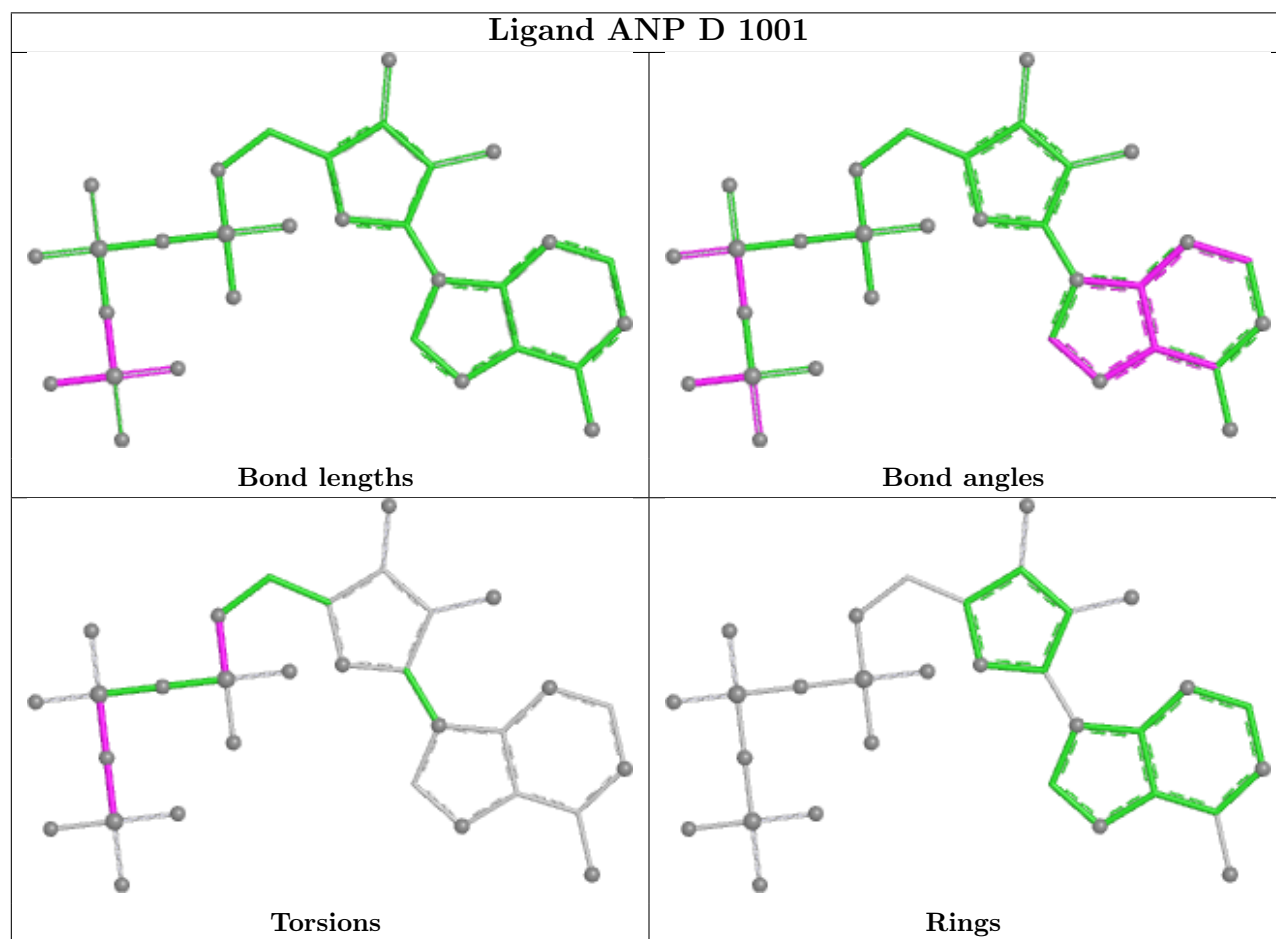
There are no ring outliers.

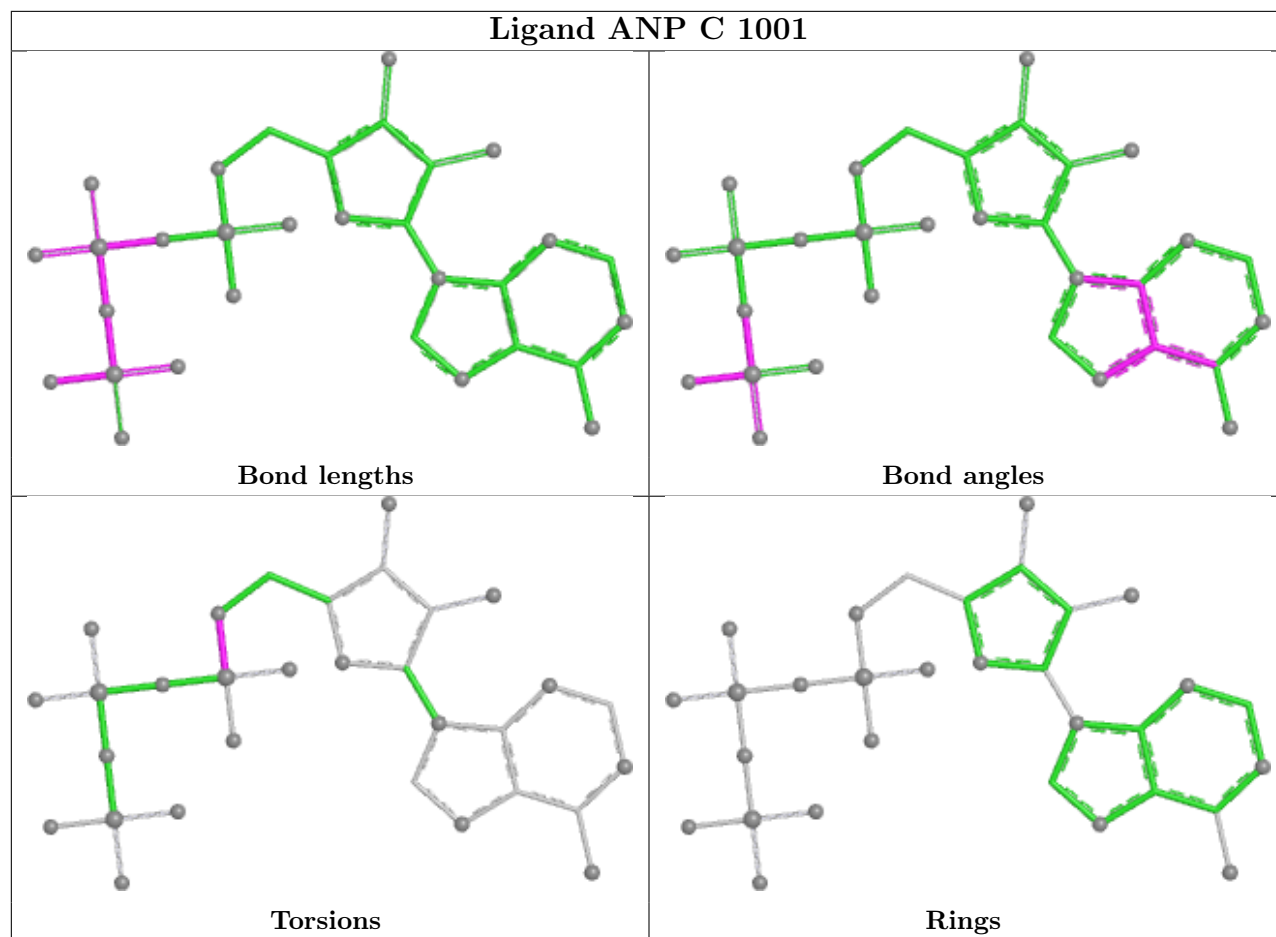
7 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	HFG	6	0
2	D	1001	ANP	4	0
4	B	1003	HFG	7	0
2	C	1001	ANP	2	0
2	A	1001	ANP	2	0
4	C	1003	HFG	6	0
4	D	1003	HFG	4	0

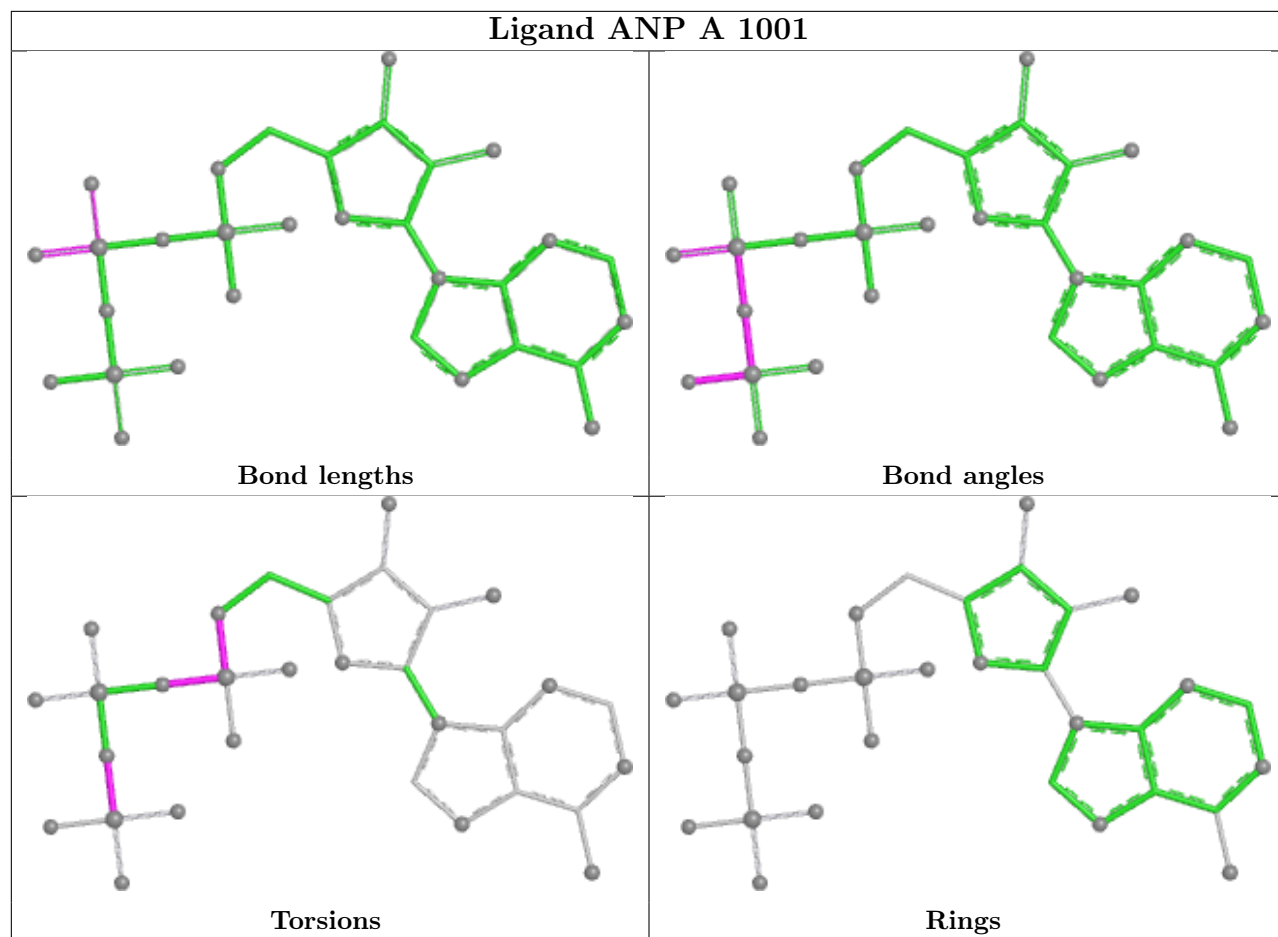
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

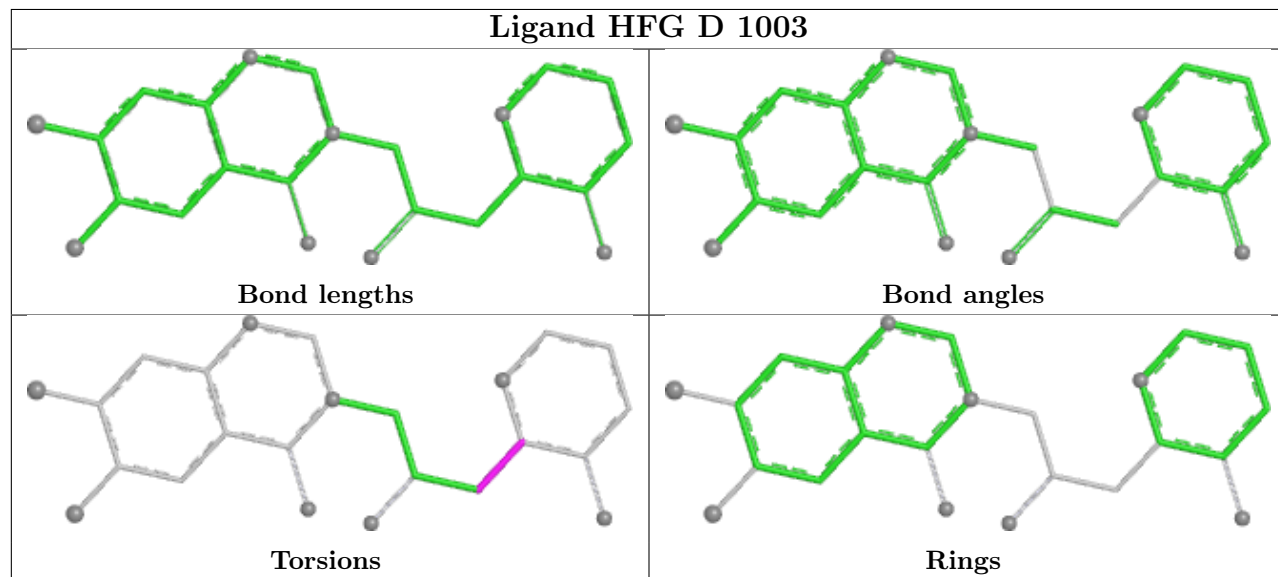


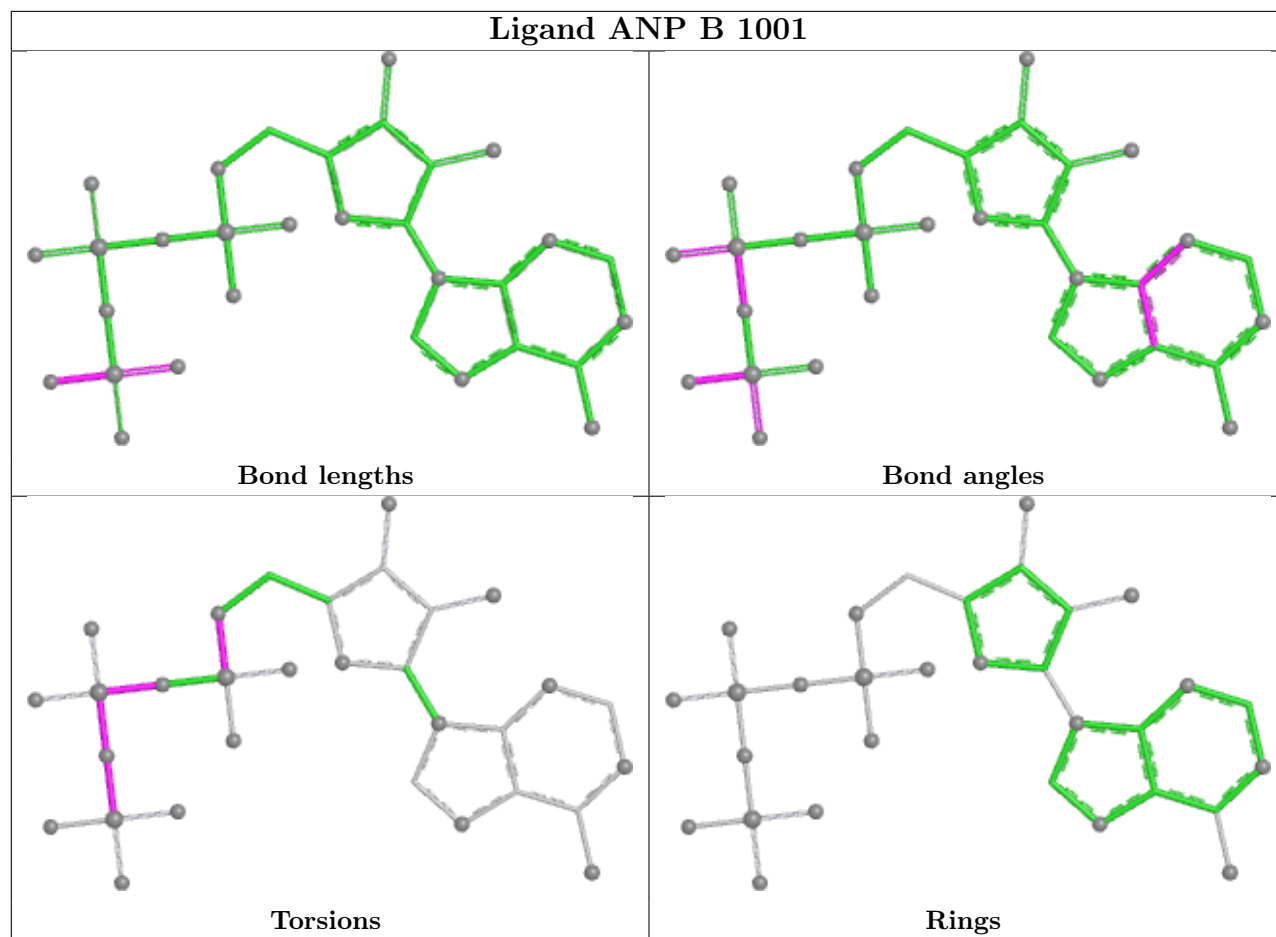


Ligand ANP A 1001



Ligand HFG D 1003





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	471/498 (94%)	-1.04	0 100 100	10, 26, 45, 59	0
1	B	475/498 (95%)	-1.04	0 100 100	9, 26, 48, 71	1 (0%)
1	C	463/498 (92%)	-0.94	0 100 100	12, 34, 69, 80	1 (0%)
1	D	457/498 (91%)	-0.96	0 100 100	11, 33, 68, 84	2 (0%)
All	All	1866/1992 (93%)	-1.00	0 100 100	9, 28, 63, 84	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HFG	D	1003	24/24	0.96	0.10	47,54,70,98	0
4	HFG	C	1003	24/24	0.97	0.09	39,51,63,84	0
2	ANP	C	1001	31/31	0.98	0.07	34,43,49,50	0
2	ANP	D	1001	31/31	0.98	0.07	36,41,44,46	0

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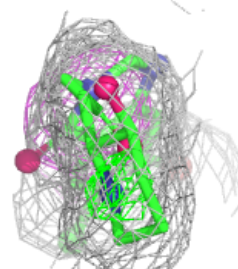
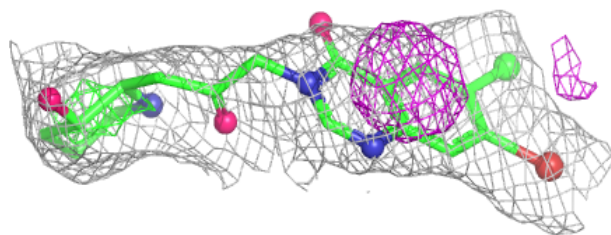
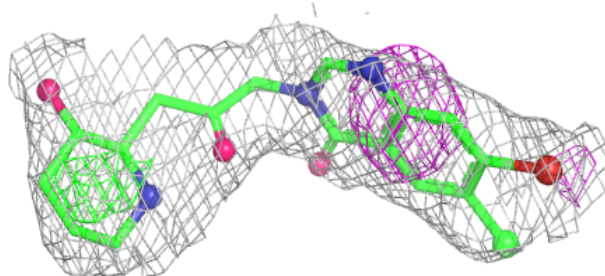
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	HFG	B	1003	24/24	0.98	0.06	29,34,48,75	0
2	ANP	A	1001	31/31	0.98	0.05	14,18,23,24	0
2	ANP	B	1001	31/31	0.98	0.05	14,20,27,28	0
3	MG	B	1002	1/1	0.99	0.03	33,33,33,33	0
3	MG	C	1002	1/1	0.99	0.03	31,31,31,31	0
4	HFG	A	1003	24/24	0.99	0.05	21,31,40,50	0
3	MG	A	1002	1/1	1.00	0.02	18,18,18,18	0
3	MG	D	1002	1/1	1.00	0.01	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.

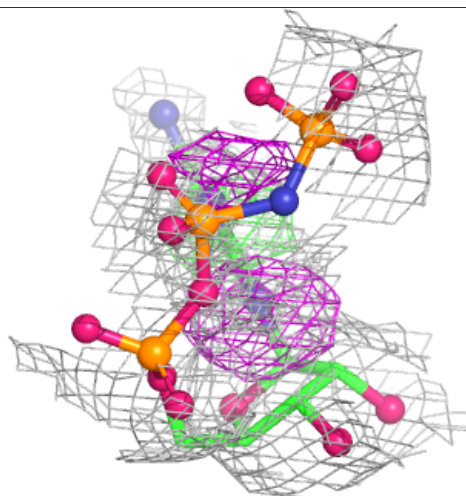
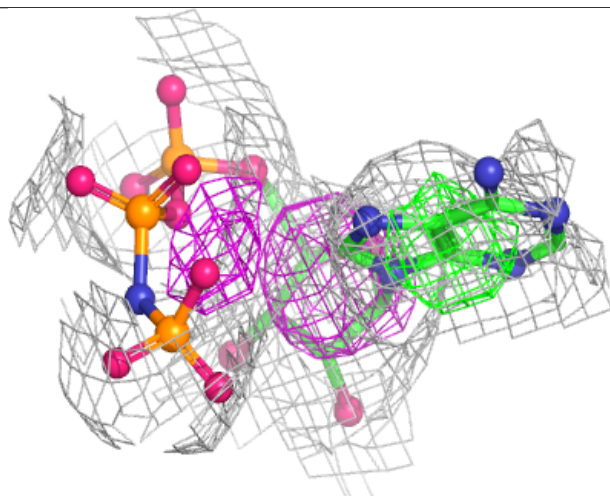
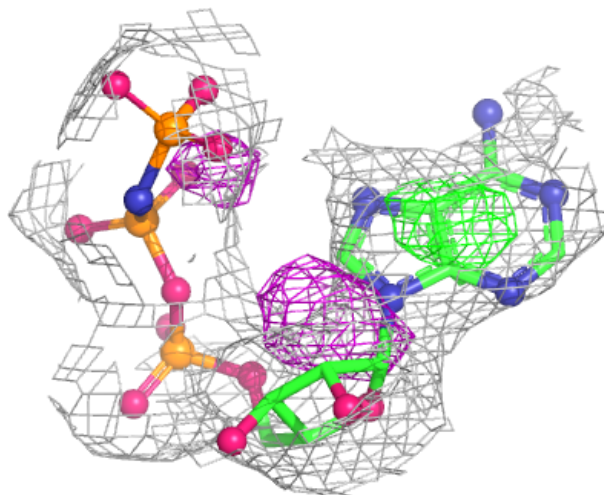
Electron density around HFG D 1003:

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



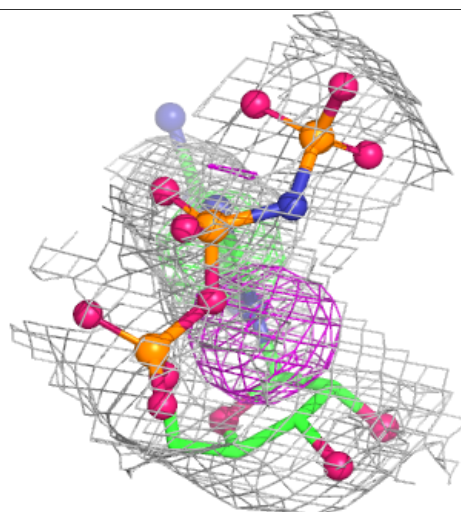
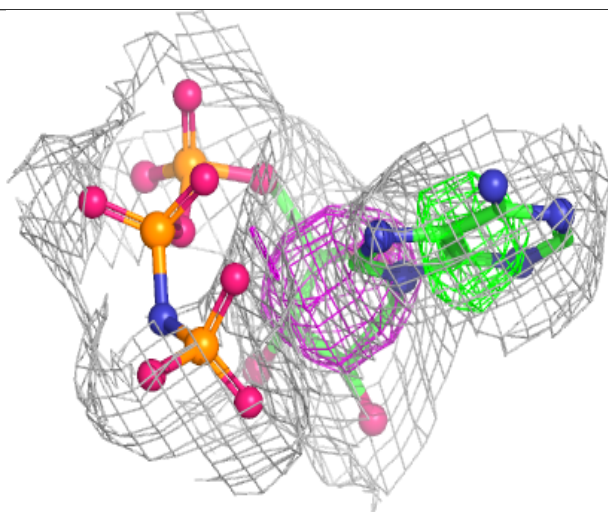
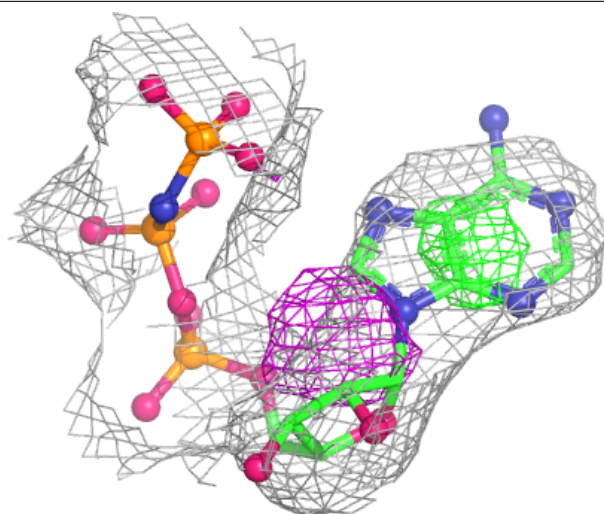
Electron density around ANP C 1001:

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



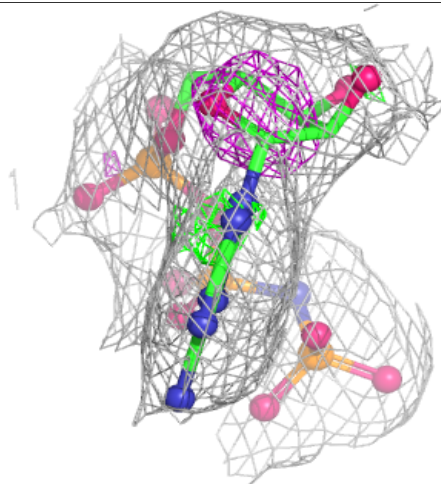
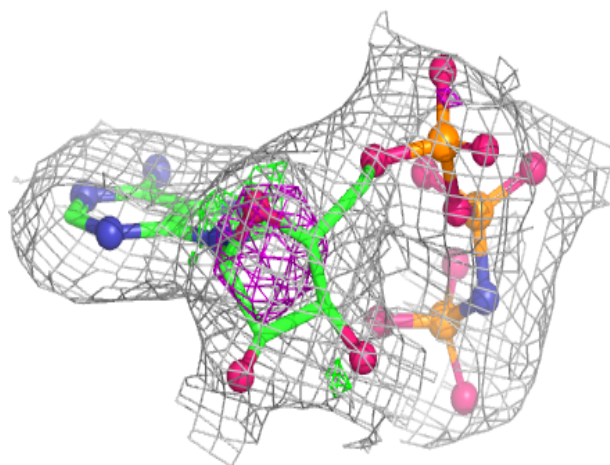
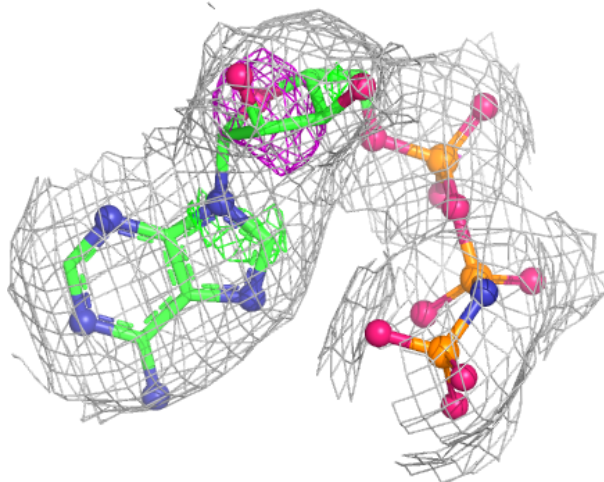
Electron density around ANP D 1001:

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



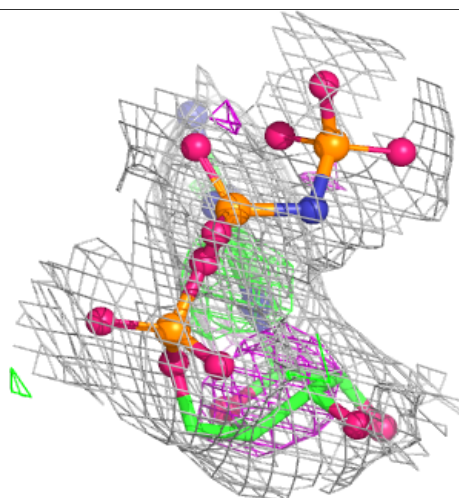
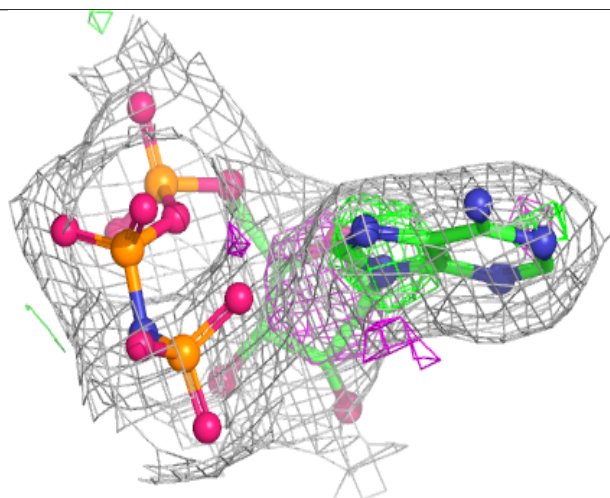
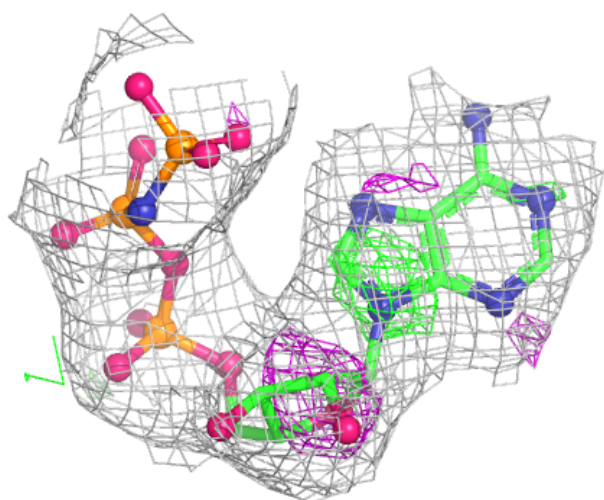
Electron density around ANP A 1001:

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



Electron density around ANP B 1001:

$2mF_o-DF_c$ (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.