



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:36 AM UTC

PDB ID : 6A88 / pdb_00006a88
Title : Crystal Structure of T. gondii prolyl tRNA synthetase with Febrifugine and ATP Analog
Authors : Kumari, S.; Mishra, S.; Yogavel, M.; Sharma, A.
Deposited on : 2018-07-06
Resolution : 2.60 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

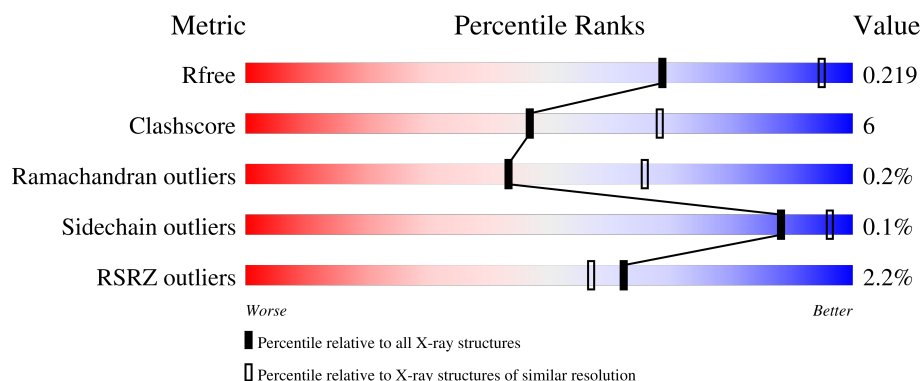
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	500	83%13%.
1	B	500	2% 83%13%.
1	C	500	4% 79%17%5%
1	D	500	82%13%5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16177 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 (ProRS).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	2	0
			3959	2543	678	716	22			
1	B	481	Total	C	N	O	S	0	0	0
			3938	2529	673	714	22			
1	C	477	Total	C	N	O	S	0	1	0
			3915	2515	671	707	22			
1	D	475	Total	C	N	O	S	0	1	0
			3893	2503	664	704	22			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	GLY	-	expression tag	UNP S8G8I1
A	332	ALA	-	expression tag	UNP S8G8I1
A	333	MET	-	expression tag	UNP S8G8I1
B	331	GLY	-	expression tag	UNP S8G8I1
B	332	ALA	-	expression tag	UNP S8G8I1
B	333	MET	-	expression tag	UNP S8G8I1
C	331	GLY	-	expression tag	UNP S8G8I1
C	332	ALA	-	expression tag	UNP S8G8I1
C	333	MET	-	expression tag	UNP S8G8I1
D	331	GLY	-	expression tag	UNP S8G8I1
D	332	ALA	-	expression tag	UNP S8G8I1
D	333	MET	-	expression tag	UNP S8G8I1

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

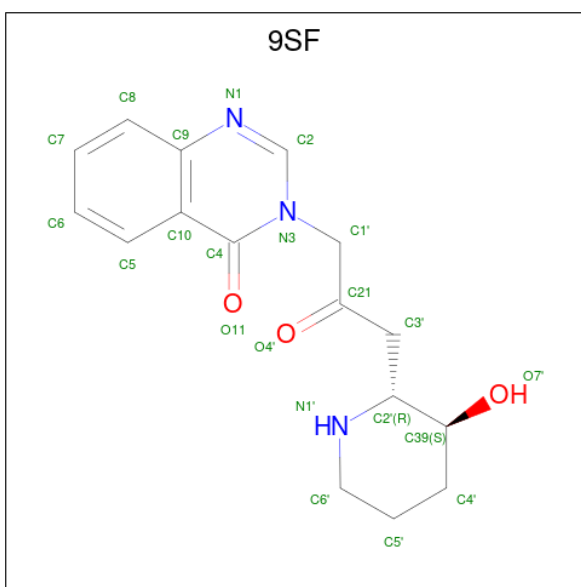


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- 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 3-{3-[(2R,3S)-3-hydroxypiperidin-2-yl]-2-oxopropyl}quinazolin-4(3H)-one (CCD ID: 9SF) (formula: C₁₆H₁₉N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			22	16	3	3		
4	B	1	Total	C	N	O	0	0
			22	16	3	3		
4	C	1	Total	C	N	O	0	0
			22	16	3	3		
4	D	1	Total	C	N	O	0	0
			22	16	3	3		

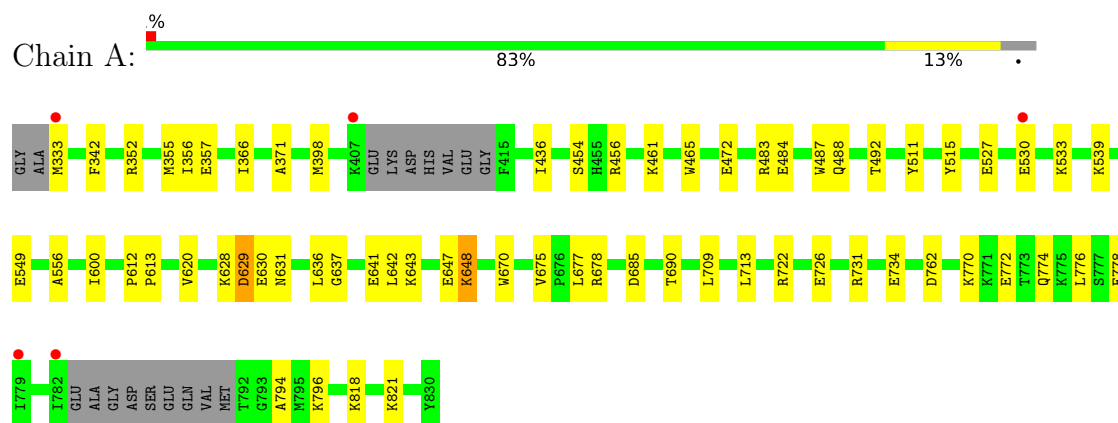
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	104	Total	O	0	0
			104	104		
5	B	53	Total	O	0	0
			53	53		
5	C	36	Total	O	0	0
			36	36		
5	D	63	Total	O	0	0
			63	63		

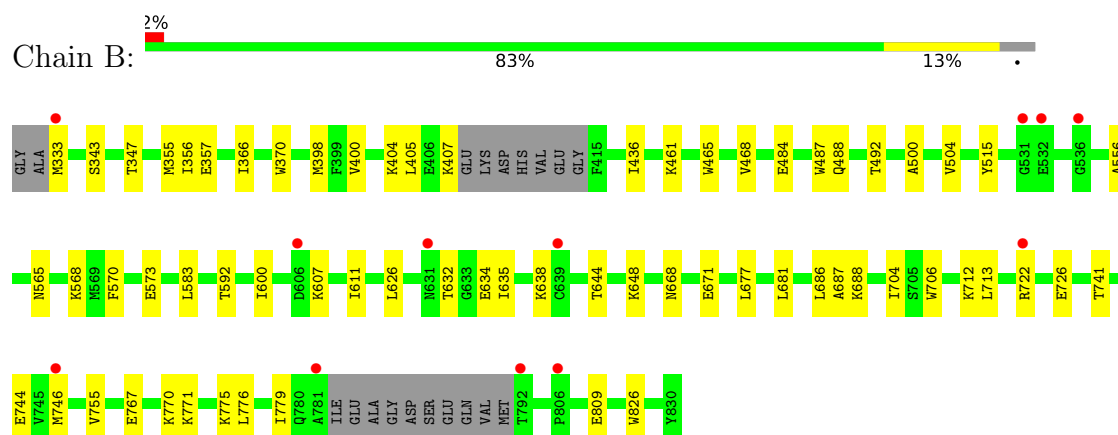
3 Residue-property plots

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.

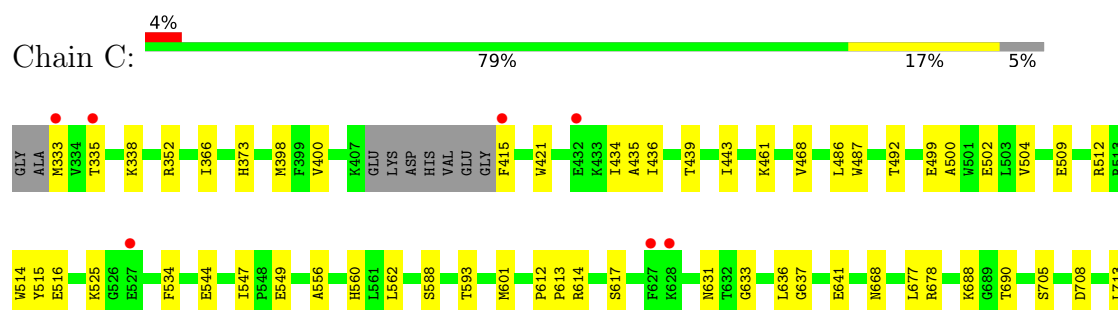
• Molecule 1: Prolyl-tRNA synthetase (ProRS)

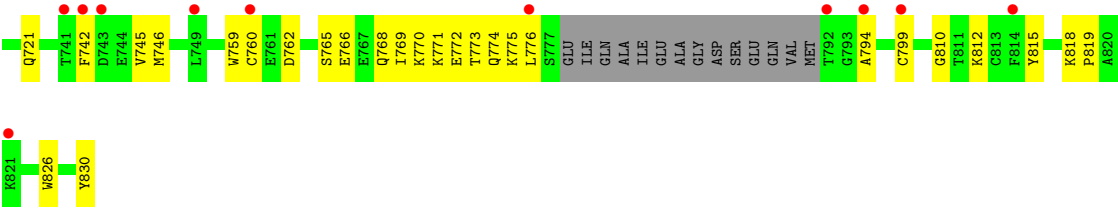


• Molecule 1: Prolyl-tRNA synthetase (ProRS)

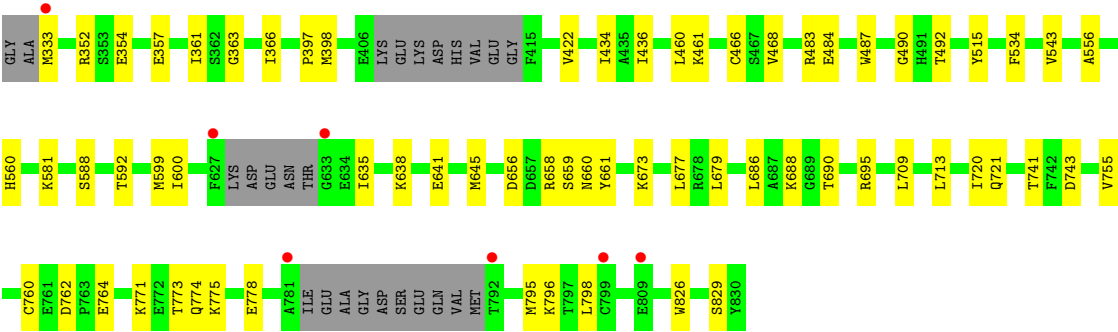
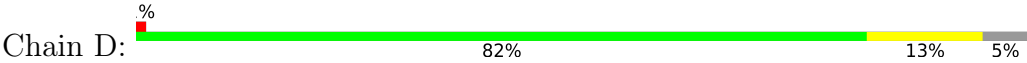


• Molecule 1: Prolyl-tRNA synthetase (ProRS)





● Molecule 1: Prolyl-tRNA synthetase (ProRS)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.91Å 90.88Å 93.03Å 89.91° 80.30° 75.58°	Depositor
Resolution (Å)	39.94 – 2.60 39.94 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.3 (39.94-2.60) 98.3 (39.94-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.15rc2_3428	Depositor
R, R_{free}	0.172 , 0.220 0.175 , 0.219	Depositor DCC
R_{free} test set	3664 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16177	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: 9SF, MG, ANP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/4071	0.44	2/5503 (0.0%)
1	B	0.16	0/4044	0.41	0/5467
1	C	0.17	0/4024	0.43	0/5439
1	D	0.17	0/4001	0.44	0/5409
All	All	0.17	0/16140	0.43	2/21818 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	630	GLU	CA-CB-CG	-5.25	103.61	114.10
1	A	629	ASP	N-CA-C	5.12	121.70	110.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3959	0	3931	42	0
1	B	3938	0	3901	46	0
1	C	3915	0	3884	52	0
1	D	3893	0	3855	47	0
2	A	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	13	0	0
2	C	31	0	13	0	0
2	D	31	0	13	0	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	22	0	0	0	0
4	B	22	0	0	0	0
4	C	22	0	0	0	0
4	D	22	0	0	0	0
5	A	104	0	0	1	0
5	B	53	0	0	0	0
5	C	36	0	0	2	0
5	D	63	0	0	0	0
All	All	16177	0	15623	180	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 6.

All (180) 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:A:355:MET:HE1	1:A:600:ILE:HD11	1.42	0.97
1:A:398:MET:HE1	1:B:398:MET:HE1	1.60	0.83
1:C:515:TYR:CZ	1:C:556:ALA:HB1	2.26	0.71
1:B:565:ASN:HA	1:B:568:LYS:HD2	1.73	0.71
1:B:515:TYR:CZ	1:B:556:ALA:HB1	2.27	0.69
1:B:355:MET:HE1	1:B:600:ILE:HD11	1.73	0.68
1:C:677:LEU:HD13	1:C:713:LEU:HD22	1.74	0.68
1:D:677:LEU:HD13	1:D:713:LEU:HD22	1.75	0.68
1:D:688:LYS:HE2	1:D:690:THR:HG21	1.75	0.68
1:B:333:MET:HG3	1:B:668:ASN:ND2	2.08	0.68
1:D:515:TYR:CZ	1:D:556:ALA:HB1	2.28	0.67
1:A:677:LEU:HD13	1:A:713:LEU:HD22	1.77	0.66
1:A:515:TYR:CZ	1:A:556:ALA:HB1	2.30	0.66
1:A:355:MET:HE3	1:A:371:ALA:HB2	1.78	0.66
1:B:767:GLU:HA	1:B:770:LYS:HG2	1.77	0.65
1:D:773:THR:HG21	1:D:795:MET:HB3	1.78	0.65
1:C:773:THR:HA	1:C:776:LEU:HD23	1.80	0.63
1:C:774:GLN:HB2	1:C:794:ALA:HB2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:HA	1:A:734:GLU:HG2	1.83	0.60
1:B:767:GLU:O	1:B:771:LYS:HG3	2.01	0.60
1:C:688:LYS:HE2	1:C:690:THR:OG1	2.01	0.60
1:C:746:MET:HE3	1:C:776:LEU:HB2	1.82	0.59
1:C:468:VAL:HG21	1:C:487:TRP:CE2	2.38	0.58
1:C:499:GLU:O	1:C:502:GLU:HG3	2.04	0.58
1:C:500:ALA:O	1:C:504:VAL:HG23	2.04	0.58
1:B:357:GLU:HB3	1:B:366:ILE:HB	1.85	0.58
1:B:355:MET:HE1	1:B:600:ILE:CD1	2.32	0.58
1:A:643:LYS:O	1:A:647:GLU:HG3	2.03	0.57
1:A:772:GLU:O	1:A:776:LEU:HG	2.06	0.56
1:D:762:ASP:HB3	1:D:764:GLU:OE2	2.06	0.56
1:B:704:ILE:HD13	1:B:712:LYS:HG2	1.88	0.56
1:C:768:GLN:NE2	1:C:815:TYR:HE2	2.04	0.55
1:B:634:GLU:HG2	1:B:686:LEU:HD21	1.88	0.55
1:D:638:LYS:HA	1:D:641:GLU:HG3	1.88	0.55
1:C:637:GLY:O	1:C:641:GLU:HG3	2.07	0.55
1:B:638:LYS:HE2	1:B:706:TRP:CE3	2.42	0.55
1:C:818:LYS:HG3	1:C:819:PRO:HD2	1.89	0.54
1:D:490:GLY:O	1:D:588:SER:HA	2.07	0.54
1:C:400:VAL:HG22	1:C:443:ILE:HD11	1.89	0.54
1:B:400:VAL:HG11	1:B:405:LEU:HD13	1.90	0.54
1:A:436:ILE:HD11	1:B:436:ILE:HD11	1.90	0.53
1:C:769:ILE:HD13	1:C:826:TRP:CH2	2.44	0.53
1:C:771:LYS:HB3	1:C:775:LYS:HZ1	1.73	0.53
1:B:407:LYS:HE2	1:B:570:PHE:CZ	2.44	0.53
1:B:573:GLU:HG2	1:B:583:LEU:HD23	1.91	0.53
1:D:333:MET:O	1:D:352:ARG:NH1	2.42	0.52
1:B:775:LYS:O	1:B:779:ILE:HG12	2.10	0.52
1:B:746:MET:SD	1:B:776:LEU:HB2	2.49	0.52
1:B:333:MET:HG3	1:B:668:ASN:HD21	1.73	0.52
1:A:530:GLU:HG2	1:A:533:LYS:HE3	1.90	0.52
1:C:631:ASN:ND2	1:C:633:GLY:H	2.08	0.52
1:D:741:THR:OG1	1:D:743:ASP:OD1	2.24	0.52
1:D:679:LEU:HD11	1:D:709:LEU:HD21	1.92	0.52
1:A:488:GLN:NE2	1:A:511:TYR:OH	2.40	0.51
1:D:461:LYS:HA	1:D:492:THR:HG22	1.92	0.51
1:D:635:ILE:HG13	1:D:686:LEU:HD12	1.92	0.51
1:D:755:VAL:HG23	1:D:826:TRP:HB2	1.94	0.50
1:C:544:GLU:HG3	1:C:799:CYS:HB3	1.94	0.50
1:A:465:TRP:CE3	1:A:488:GLN:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:LYS:HE2	1:B:706:TRP:CD2	2.48	0.49
1:A:484:GLU:CD	1:B:398:MET:HG2	2.37	0.49
1:A:642:LEU:HD22	1:A:709:LEU:HD12	1.94	0.49
1:C:509:GLU:OE1	1:C:525:LYS:NZ	2.40	0.49
1:A:774:GLN:O	1:A:778:GLU:HG3	2.13	0.49
1:B:468:VAL:HG21	1:B:487:TRP:CE2	2.48	0.49
1:B:607:LYS:HE2	1:B:671:GLU:OE2	2.12	0.49
1:C:759:TRP:CD1	1:C:760:CYS:H	2.31	0.49
1:A:731:ARG:O	1:A:734:GLU:HG2	2.13	0.48
1:B:635:ILE:HG23	1:B:681:LEU:HD22	1.94	0.48
1:D:771:LYS:HA	1:D:774:GLN:HG2	1.96	0.48
1:B:404:LYS:O	1:B:407:LYS:NZ	2.45	0.48
1:C:338:LYS:HG2	1:C:549:GLU:HG2	1.95	0.48
1:D:460:LEU:O	1:D:492:THR:HA	2.14	0.48
1:B:687:ALA:HB3	1:B:688:LYS:NZ	2.29	0.48
1:C:436:ILE:HD11	1:D:436:ILE:HD11	1.96	0.48
1:C:772:GLU:HG3	1:C:773:THR:N	2.28	0.48
1:D:762:ASP:HB3	1:D:764:GLU:CD	2.38	0.48
1:B:487:TRP:HB3	1:B:592:THR:HG22	1.95	0.48
1:D:760:CYS:SG	1:D:762:ASP:HB2	2.54	0.48
1:A:527:GLU:CD	1:A:539:LYS:HE3	2.39	0.48
1:C:762:ASP:O	1:C:765:SER:OG	2.24	0.47
1:B:626:LEU:HD22	1:B:632:THR:HA	1.96	0.47
1:A:637:GLY:O	1:A:641:GLU:HG3	2.14	0.47
1:C:810:GLY:O	1:C:812:LYS:HE3	2.14	0.47
1:D:755:VAL:CG2	1:D:826:TRP:HB2	2.45	0.47
1:A:398:MET:HG2	1:B:484:GLU:CD	2.39	0.47
1:A:631:ASN:ND2	1:A:636:LEU:HD12	2.30	0.47
1:C:614:ARG:HH21	1:C:721:GLN:HG2	1.80	0.47
1:C:512:ARG:HD3	1:C:525:LYS:HE3	1.95	0.47
1:A:472:GLU:H	1:A:483:ARG:HD3	1.80	0.47
1:D:543:VAL:HG23	1:D:556:ALA:HB3	1.97	0.47
1:B:677:LEU:HD13	1:B:713:LEU:HD22	1.96	0.47
1:C:742:PHE:O	1:C:745:VAL:HG13	2.14	0.47
1:B:573:GLU:HG2	1:B:583:LEU:CD2	2.45	0.46
1:D:357:GLU:HB3	1:D:366:ILE:HB	1.96	0.46
1:A:631:ASN:HD21	1:A:636:LEU:HD12	1.81	0.46
1:A:770:LYS:HD2	1:A:796:LYS:HB3	1.96	0.46
1:C:415:PHE:N	5:C:1103:HOH:O	2.48	0.46
1:B:465:TRP:CE3	1:B:488:GLN:HB3	2.50	0.46
1:A:620:VAL:HG21	1:A:713:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:366:ILE:HG12	1:D:397:PRO:HD3	1.97	0.46
1:D:688:LYS:HG2	1:D:690:THR:HG23	1.97	0.46
1:C:333:MET:HE3	1:C:668:ASN:OD1	2.16	0.46
1:C:335:THR:HG23	1:C:352:ARG:HH12	1.81	0.46
1:C:486:LEU:HB2	1:C:593:THR:HG23	1.98	0.45
1:C:562:LEU:HD11	1:C:588:SER:HB3	1.99	0.45
1:A:648:LYS:HD3	1:A:648:LYS:HA	1.54	0.45
1:D:645:MET:HE3	1:D:645:MET:HB3	1.90	0.45
1:D:709:LEU:HD12	1:D:709:LEU:HA	1.85	0.45
1:A:487:TRP:C	1:A:487:TRP:CD1	2.95	0.45
1:D:487:TRP:C	1:D:487:TRP:CD1	2.95	0.45
1:D:656:ASP:OD1	1:D:658:ARG:HB2	2.17	0.45
1:D:774:GLN:O	1:D:778:GLU:HG2	2.17	0.44
1:A:774:GLN:HG2	1:A:794:ALA:HB2	1.98	0.44
1:C:373:HIS:CE1	1:C:617:SER:HA	2.52	0.44
1:D:534:PHE:HB2	1:D:560:HIS:CE1	2.52	0.44
1:B:461:LYS:HA	1:B:492:THR:HG22	1.98	0.44
1:C:547:ILE:HD12	1:C:830:TYR:CE2	2.53	0.44
1:C:705:SER:OG	1:C:708:ASP:OD2	2.36	0.44
1:D:774:GLN:HG3	1:D:775:LYS:N	2.32	0.44
1:D:659:SER:O	1:D:661:TYR:N	2.51	0.43
1:A:722:ARG:HG2	1:A:726:GLU:OE2	2.19	0.43
1:D:677:LEU:HD23	1:D:695:ARG:HA	1.99	0.43
1:A:762:ASP:OD2	1:A:818:LYS:NZ	2.50	0.43
1:C:512:ARG:NH1	1:C:516:GLU:OE1	2.50	0.43
1:A:454:SER:OG	1:A:456:ARG:HG3	2.19	0.43
1:C:487:TRP:C	1:C:487:TRP:CD1	2.96	0.43
1:C:612:PRO:HA	1:C:613:PRO:HD3	1.93	0.43
1:D:363:GLY:HA3	1:D:483:ARG:HG3	2.00	0.43
1:D:466:CYS:SG	1:D:487:TRP:NE1	2.87	0.43
1:B:487:TRP:CB	1:B:592:THR:HG22	2.48	0.43
1:B:722:ARG:O	1:B:726:GLU:HG2	2.18	0.43
1:B:809:GLU:H	1:B:809:GLU:CD	2.27	0.43
1:A:678:ARG:HD3	5:A:1138:HOH:O	2.19	0.42
1:B:487:TRP:CD1	1:B:487:TRP:C	2.97	0.42
1:C:636:LEU:HD12	1:C:636:LEU:HA	1.87	0.42
1:C:678:ARG:HD3	5:C:1120:HOH:O	2.20	0.42
1:A:342:PHE:CD1	1:A:549:GLU:HG2	2.55	0.42
1:A:356:ILE:HA	1:A:366:ILE:O	2.19	0.42
1:C:434:ILE:HD13	1:D:361:ILE:HD13	2.00	0.42
1:C:765:SER:O	1:C:768:GLN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:766:GLU:HG2	1:C:770:LYS:HD3	2.00	0.42
1:C:398:MET:HE1	1:D:398:MET:SD	2.59	0.42
1:C:421:TRP:CZ3	1:C:435:ALA:HB2	2.54	0.42
1:D:581:LYS:HB3	1:D:581:LYS:HE3	1.71	0.42
1:D:771:LYS:O	1:D:774:GLN:HG2	2.19	0.42
1:D:599:MET:HE2	1:D:600:ILE:HG13	2.01	0.42
1:D:798:LEU:HD21	1:D:829:SER:HB3	2.01	0.42
1:D:659:SER:C	1:D:661:TYR:H	2.28	0.42
1:B:741:THR:HG22	1:B:744:GLU:OE1	2.20	0.42
1:C:333:MET:O	1:C:352:ARG:NH1	2.53	0.41
1:C:514:TRP:C	1:C:514:TRP:CD1	2.98	0.41
1:D:720:ILE:O	1:D:721:GLN:C	2.63	0.41
1:A:461:LYS:HA	1:A:492:THR:HG22	2.02	0.41
1:A:670:TRP:CE3	1:A:675:VAL:HG21	2.56	0.41
1:B:644:THR:HG23	1:B:648:LYS:HE3	2.02	0.41
1:B:746:MET:HE2	1:B:746:MET:HB3	1.95	0.41
1:C:461:LYS:HA	1:C:492:THR:HG22	2.01	0.41
1:C:547:ILE:HD13	1:C:601:MET:SD	2.60	0.41
1:D:422:VAL:HB	1:D:434:ILE:HG12	2.03	0.41
1:D:487:TRP:CB	1:D:592:THR:HG22	2.51	0.41
2:A:1001:ANP:O3G	2:A:1001:ANP:O2B	2.38	0.41
1:C:534:PHE:HB2	1:C:560:HIS:CE1	2.56	0.41
1:A:549:GLU:N	1:A:549:GLU:OE2	2.53	0.41
1:B:687:ALA:HB3	1:B:688:LYS:HZ3	1.86	0.41
1:A:515:TYR:CE2	1:A:556:ALA:HB1	2.56	0.41
1:A:612:PRO:HA	1:A:613:PRO:HD3	1.94	0.41
1:A:685:ASP:HB3	1:A:690:THR:O	2.21	0.41
1:B:343:SER:O	1:B:347:THR:HG23	2.21	0.41
1:B:755:VAL:CG2	1:B:826:TRP:HB2	2.50	0.41
1:C:768:GLN:HE21	1:C:815:TYR:HE2	1.67	0.41
1:A:821:LYS:HE2	1:A:821:LYS:HB3	1.80	0.41
1:B:370:TRP:HE1	1:B:611:ILE:HD11	1.86	0.41
1:B:500:ALA:O	1:B:504:VAL:HG23	2.21	0.41
1:A:333:MET:O	1:A:352:ARG:NH1	2.53	0.40
1:D:468:VAL:O	1:D:484:GLU:HA	2.21	0.40
1:A:357:GLU:HB3	1:A:366:ILE:HB	2.03	0.40
1:D:354:GLU:OE1	1:D:673:LYS:NZ	2.54	0.40
1:D:796:LYS:HD3	1:D:829:SER:OG	2.22	0.40
1:B:356:ILE:HD13	1:B:356:ILE:HA	1.90	0.40

There are no symmetry-related clashes.

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	478/500 (96%)	464 (97%)	13 (3%)	1 (0%)	43	66
1	B	475/500 (95%)	460 (97%)	15 (3%)	0	100	100
1	C	472/500 (94%)	455 (96%)	16 (3%)	1 (0%)	43	66
1	D	468/500 (94%)	455 (97%)	12 (3%)	1 (0%)	43	66
All	All	1893/2000 (95%)	1834 (97%)	56 (3%)	3 (0%)	43	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	629	ASP
1	C	439	THR
1	D	660	ASN

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	425/436 (98%)	423 (100%)	2 (0%)	81	92
1	B	422/436 (97%)	422 (100%)	0	100	100
1	C	420/436 (96%)	420 (100%)	0	100	100
1	D	417/436 (96%)	417 (100%)	0	100	100
All	All	1684/1744 (97%)	1682 (100%)	2 (0%)	88	96

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

Mol	Chain	Res	Type
1	A	628	LYS
1	A	648	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	585	HIS
1	A	631	ASN
1	A	750	ASN
1	A	768	GLN
1	A	780	GLN
1	B	341	ASN
1	B	455	HIS
1	B	586	GLN
1	B	669	HIS
1	B	768	GLN
1	C	341	ASN
1	C	488	GLN
1	C	555	GLN
1	C	580	HIS
1	C	585	HIS
1	C	631	ASN
1	C	750	ASN
1	C	768	GLN
1	D	341	ASN
1	D	403	HIS
1	D	488	GLN
1	D	750	ASN
1	D	780	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	9SF	D	1003	-	24,24,24	0.86	0	25,33,33	1.61	1 (4%)
4	9SF	C	1003	-	24,24,24	1.00	1 (4%)	25,33,33	1.09	1 (4%)
2	ANP	D	1001	3	33,33,33	0.94	4 (12%)	45,52,52	0.69	1 (2%)
2	ANP	A	1001	3	33,33,33	0.94	4 (12%)	45,52,52	0.73	2 (4%)
2	ANP	B	1001	3	33,33,33	0.92	3 (9%)	45,52,52	0.63	0
4	9SF	B	1003	-	24,24,24	1.35	1 (4%)	25,33,33	0.53	0
2	ANP	C	1001	3	33,33,33	0.96	5 (15%)	45,52,52	0.78	2 (4%)
4	9SF	A	1003	-	24,24,24	0.37	0	25,33,33	0.49	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
4	9SF	D	1003	-	-	0/8/19/19	0/3/3/3
4	9SF	C	1003	-	-	0/8/19/19	0/3/3/3
2	ANP	D	1001	3	-	7/18/38/38	0/3/3/3
2	ANP	A	1001	3	-	7/18/38/38	0/3/3/3
2	ANP	B	1001	3	-	5/18/38/38	0/3/3/3
4	9SF	B	1003	-	-	0/8/19/19	0/3/3/3
2	ANP	C	1001	3	-	6/18/38/38	0/3/3/3
4	9SF	A	1003	-	-	1/8/19/19	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1003	9SF	C1'-C21	-5.01	1.45	1.51
4	C	1003	9SF	C1'-C21	-2.89	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	ANP	PG-N3B	2.68	1.70	1.63
2	C	1001	ANP	PG-N3B	2.66	1.70	1.63
2	C	1001	ANP	PG-O1G	2.59	1.50	1.46
2	D	1001	ANP	PG-N3B	2.57	1.70	1.63
2	D	1001	ANP	PG-O1G	2.56	1.50	1.46
2	B	1001	ANP	PG-O1G	2.56	1.50	1.46
2	B	1001	ANP	PG-N3B	2.55	1.70	1.63
2	A	1001	ANP	PG-O1G	2.52	1.50	1.46
2	C	1001	ANP	PB-O1B	2.49	1.50	1.46
2	B	1001	ANP	PB-O1B	2.45	1.49	1.46
2	D	1001	ANP	PB-O1B	2.32	1.49	1.46
2	A	1001	ANP	PB-O1B	2.21	1.49	1.46
2	D	1001	ANP	PB-O3A	-2.18	1.56	1.59
2	A	1001	ANP	PB-N3B	2.10	1.68	1.63
2	C	1001	ANP	PB-O3A	-2.06	1.56	1.59
2	C	1001	ANP	PB-N3B	2.04	1.68	1.63

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1003	9SF	C6'-N1'-C2'	-7.56	106.90	111.62
4	C	1003	9SF	C6'-N1'-C2'	-5.13	108.42	111.62
2	D	1001	ANP	O1G-PG-N3B	-2.30	108.38	111.77
2	A	1001	ANP	O1G-PG-N3B	-2.29	108.40	111.77
2	C	1001	ANP	O1B-PB-N3B	-2.04	108.76	111.77
2	C	1001	ANP	C3'-C2'-C1'	2.03	105.31	101.46
2	A	1001	ANP	O1B-PB-N3B	-2.01	108.81	111.77

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	ANP	PB-N3B-PG-O1G
2	A	1001	ANP	PG-N3B-PB-O1B
2	A	1001	ANP	C5'-O5'-PA-O1A
2	B	1001	ANP	PB-N3B-PG-O1G
2	B	1001	ANP	C5'-O5'-PA-O1A
2	B	1001	ANP	C5'-O5'-PA-O3A
2	C	1001	ANP	PB-N3B-PG-O1G
2	C	1001	ANP	PG-N3B-PB-O1B
2	C	1001	ANP	C5'-O5'-PA-O1A
2	C	1001	ANP	C5'-O5'-PA-O3A

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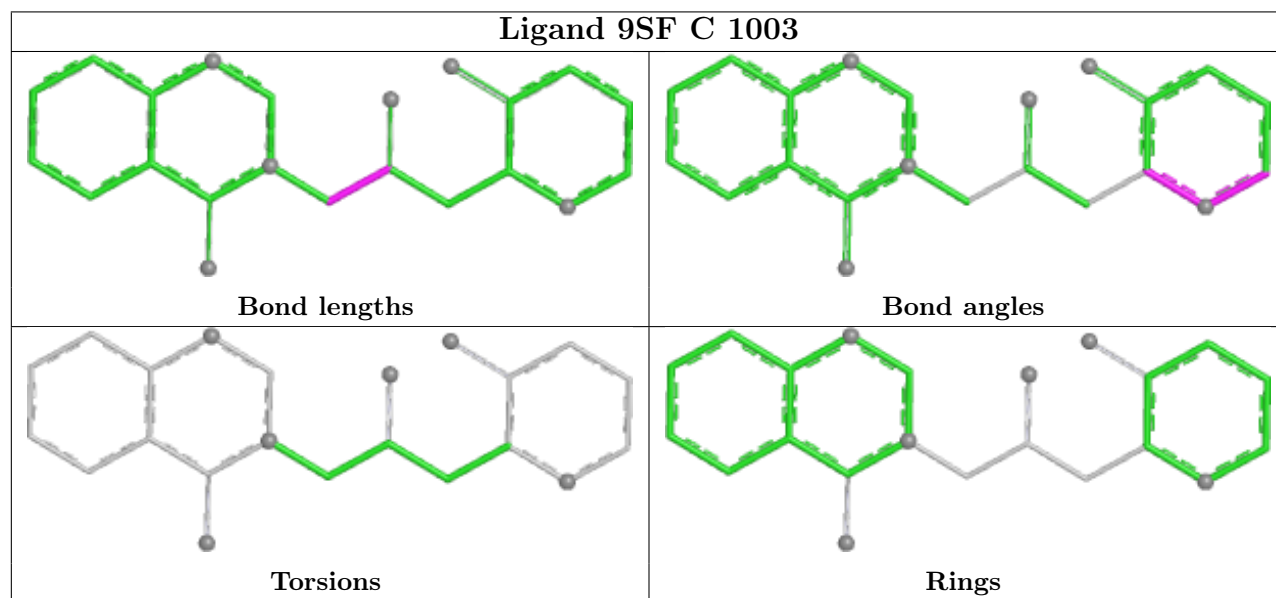
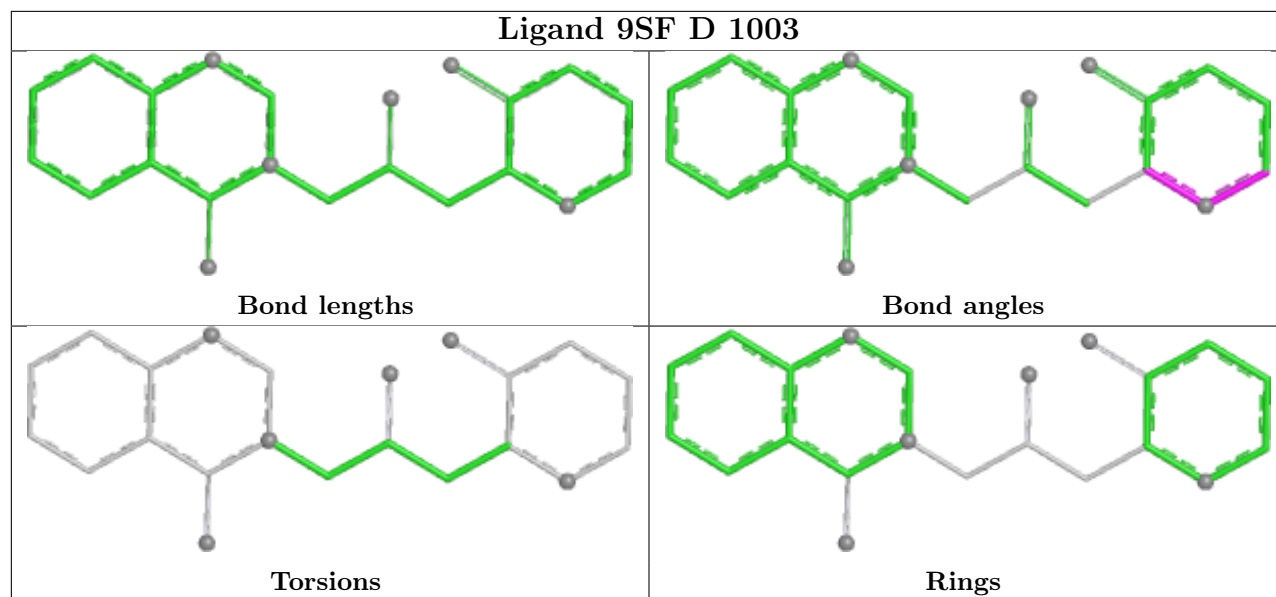
Mol	Chain	Res	Type	Atoms
2	D	1001	ANP	PB-N3B-PG-O1G
2	D	1001	ANP	PG-N3B-PB-O1B
2	D	1001	ANP	PA-O3A-PB-O1B
2	D	1001	ANP	C5'-O5'-PA-O1A
2	D	1001	ANP	C5'-O5'-PA-O3A
4	A	1003	9SF	N3-C1'-C21-O4'
2	A	1001	ANP	C5'-O5'-PA-O2A
2	A	1001	ANP	C5'-O5'-PA-O3A
2	B	1001	ANP	C5'-O5'-PA-O2A
2	C	1001	ANP	C5'-O5'-PA-O2A
2	D	1001	ANP	C5'-O5'-PA-O2A
2	D	1001	ANP	C4'-C5'-O5'-PA
2	A	1001	ANP	C4'-C5'-O5'-PA
2	A	1001	ANP	O4'-C4'-C5'-O5'
2	B	1001	ANP	C4'-C5'-O5'-PA
2	C	1001	ANP	O4'-C4'-C5'-O5'

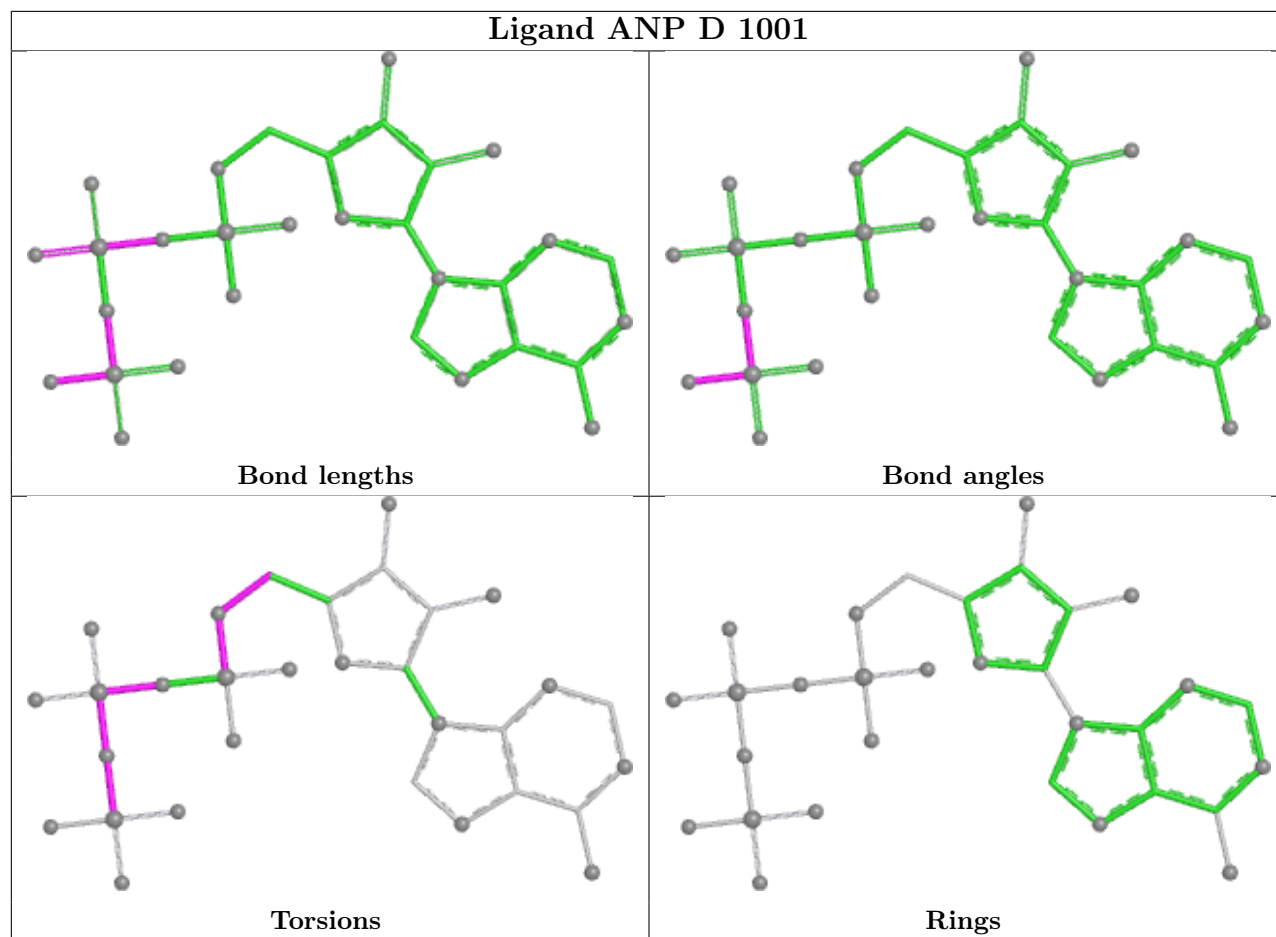
There are no ring outliers.

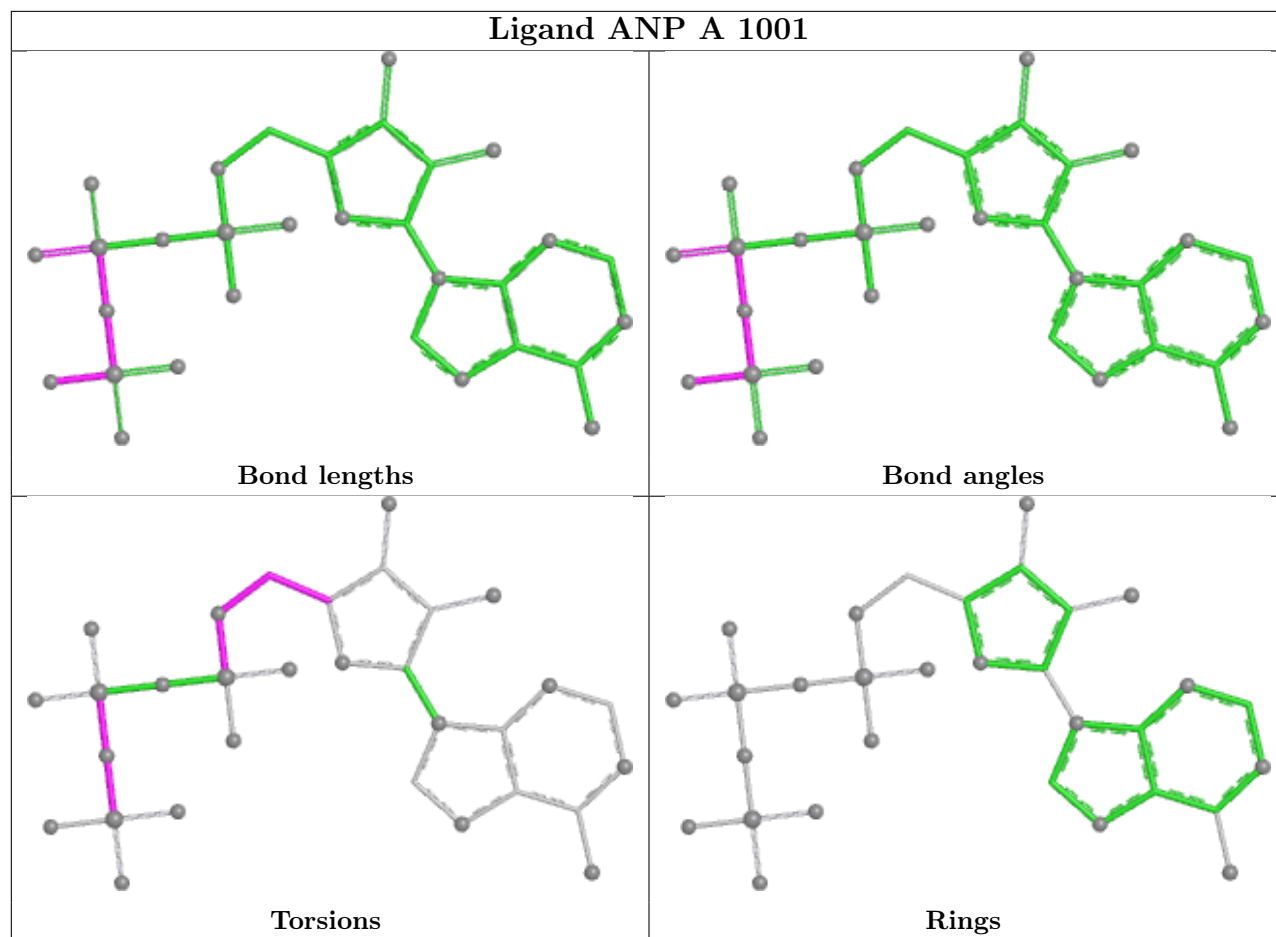
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ANP	1	0

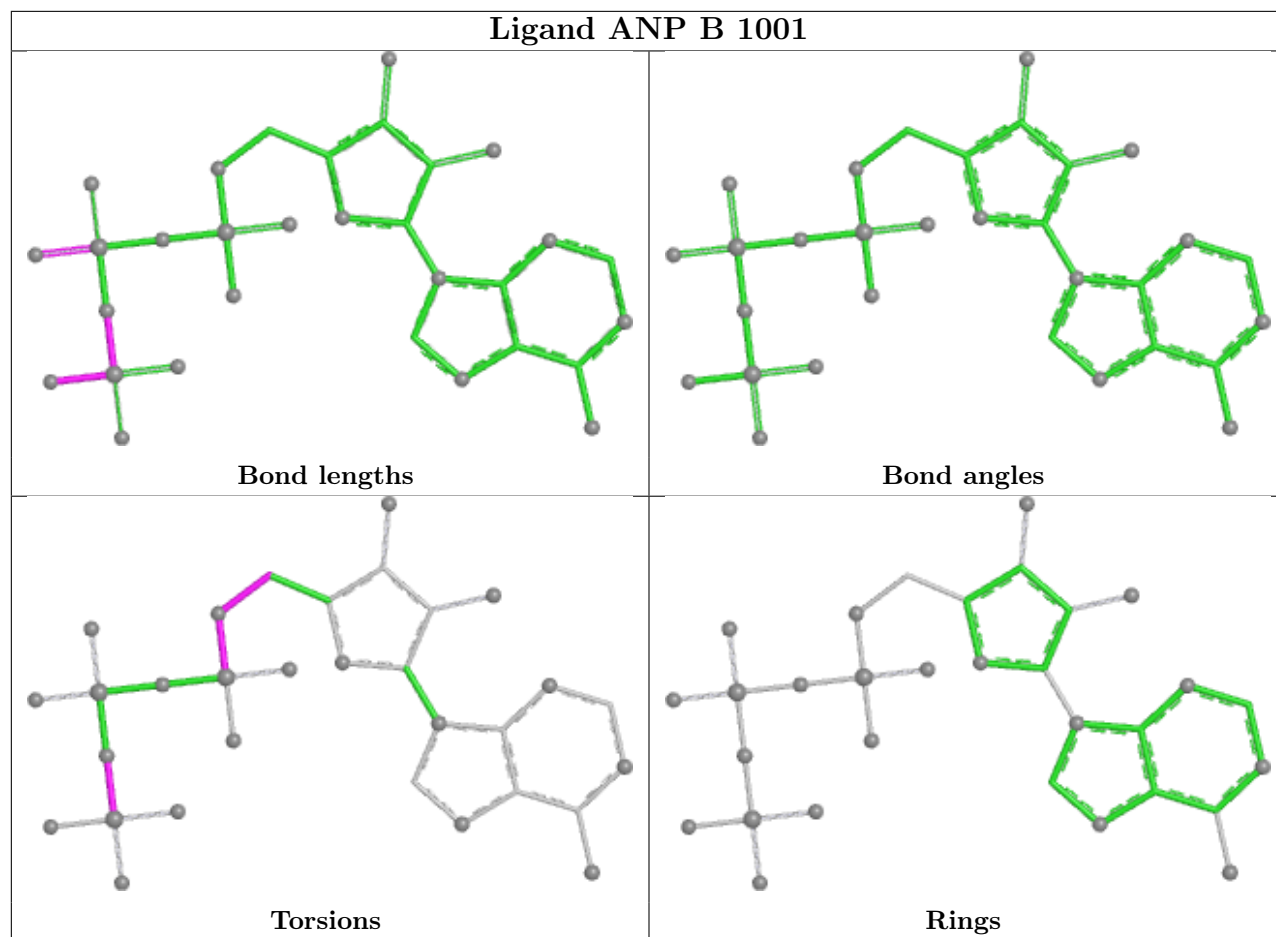
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



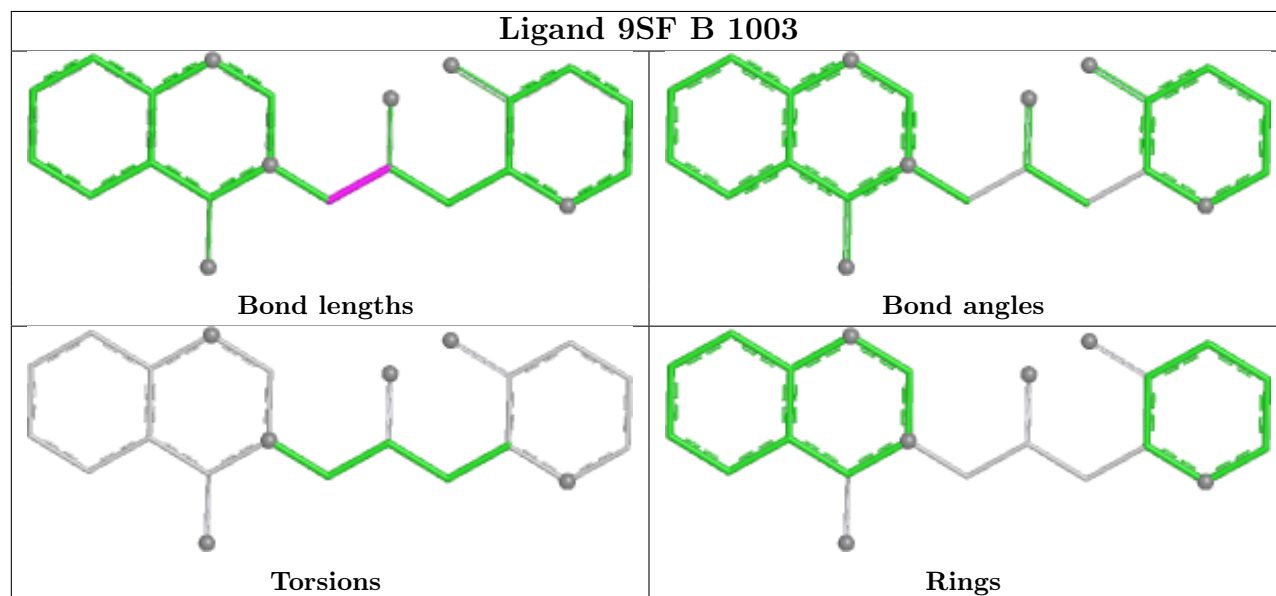


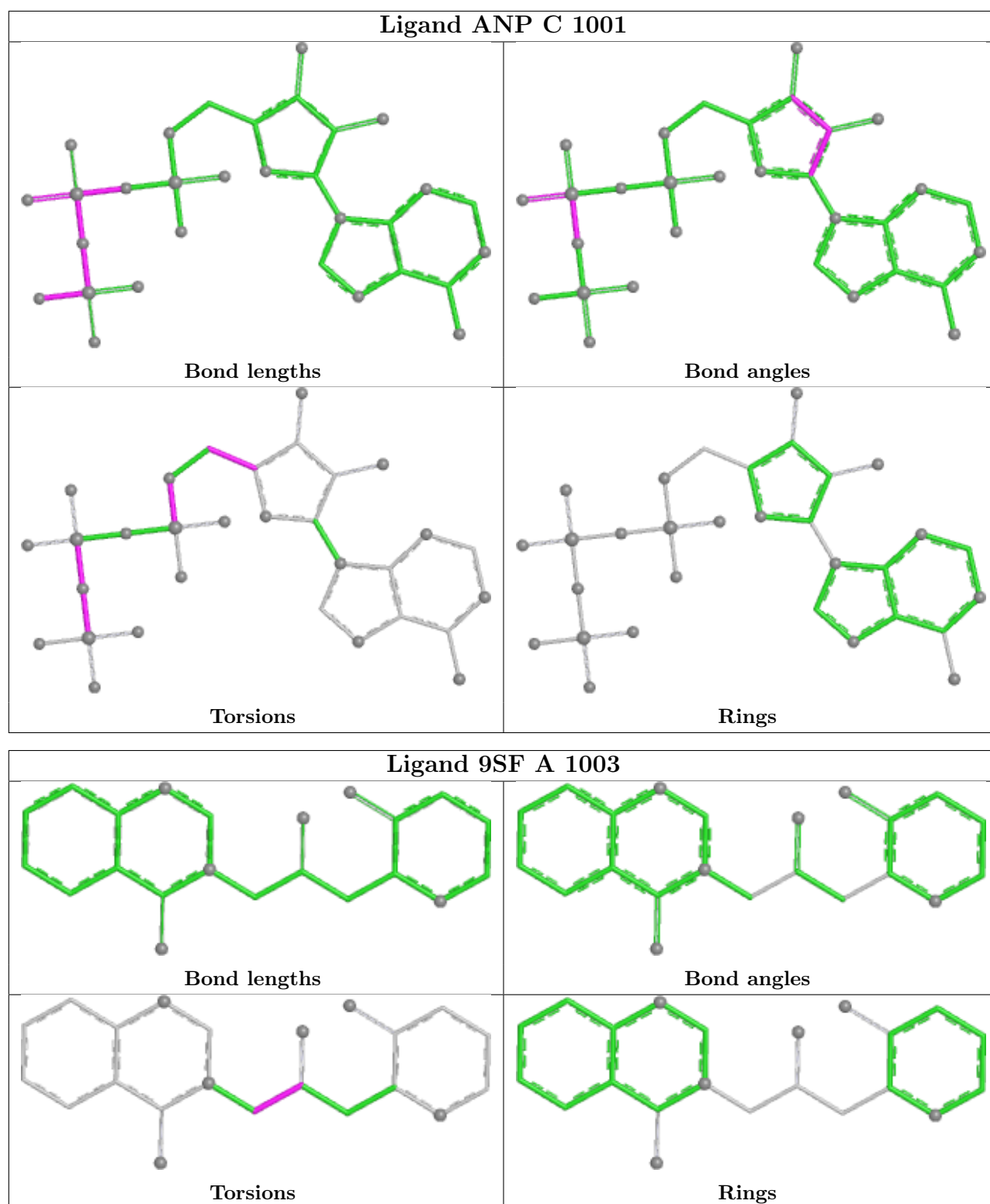


Ligand ANP B 1001



Ligand 9SF B 1003





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	482/500 (96%)	-0.16	5 (1%) 79 76	17, 36, 65, 110	3 (0%)
1	B	481/500 (96%)	0.15	12 (2%) 58 52	23, 46, 79, 97	0
1	C	477/500 (95%)	0.18	18 (3%) 44 38	22, 47, 89, 106	1 (0%)
1	D	475/500 (95%)	0.01	7 (1%) 72 68	20, 43, 73, 96	2 (0%)
All	All	1915/2000 (95%)	0.05	42 (2%) 62 57	17, 43, 79, 110	6 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	627	PHE	4.4
1	B	781	ALA	4.4
1	D	781	ALA	4.1
1	C	792	THR	3.5
1	B	792	THR	3.5
1	D	799	CYS	3.2
1	A	782	ILE	2.9
1	D	792	THR	2.9
1	C	776	LEU	2.8
1	B	532	GLU	2.8
1	C	415	PHE	2.7
1	C	799	CYS	2.7
1	A	779	ILE	2.7
1	C	743	ASP	2.6
1	C	814	PHE	2.6
1	C	527	GLU	2.6
1	B	536	GLY	2.6
1	B	333	MET	2.5
1	A	530	GLU	2.4
1	B	639	CYS	2.4
1	C	760	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	407	LYS	2.4
1	C	335	THR	2.3
1	C	741	THR	2.2
1	B	746	MET	2.2
1	C	333	MET	2.2
1	B	606	ASP	2.2
1	C	628	LYS	2.2
1	B	631	ASN	2.2
1	B	531	GLY	2.2
1	B	722	ARG	2.2
1	A	333	MET	2.1
1	D	333	MET	2.1
1	C	749	LEU	2.1
1	D	809	GLU	2.1
1	C	742	PHE	2.1
1	D	633	GLY	2.1
1	C	432	GLU	2.1
1	C	821	LYS	2.1
1	B	806	PRO	2.1
1	C	627	PHE	2.0
1	C	794	ALA	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.

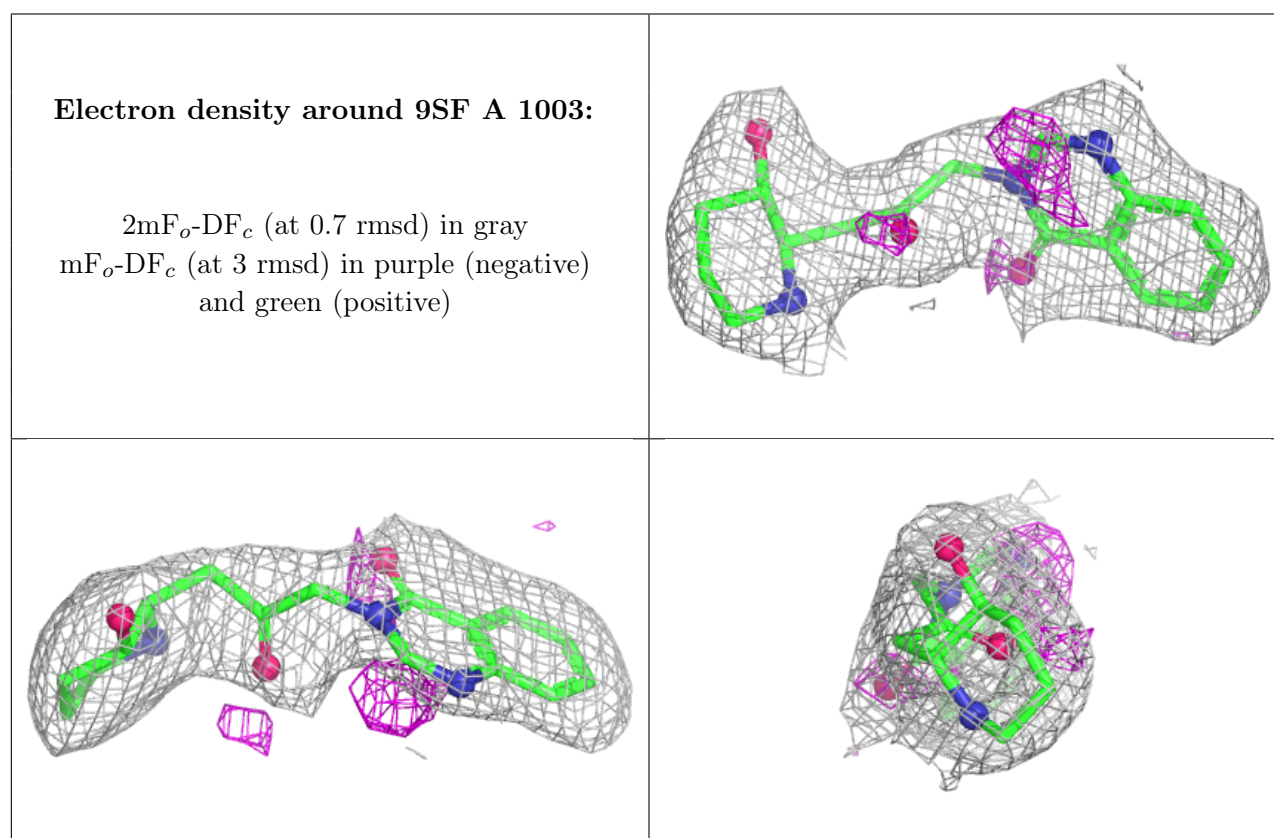
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	9SF	A	1003	22/22	0.92	0.10	22,33,36,38	0
3	MG	A	1002	1/1	0.94	0.11	29,29,29,29	0

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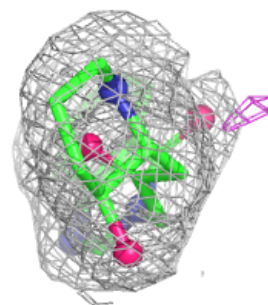
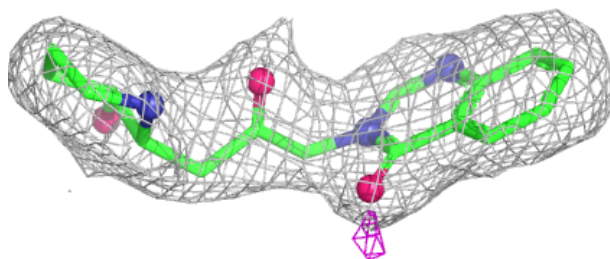
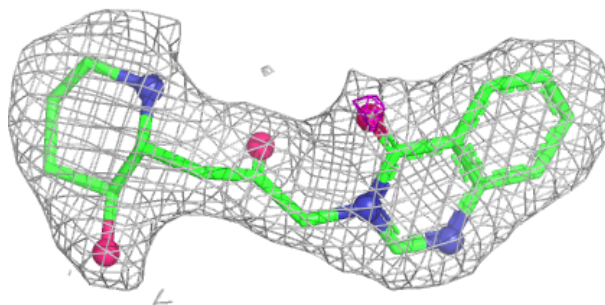
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	9SF	C	1003	22/22	0.95	0.07	30,35,40,43	0
4	9SF	B	1003	22/22	0.96	0.07	25,34,41,42	0
4	9SF	D	1003	22/22	0.96	0.06	22,30,35,39	0
2	ANP	C	1001	31/31	0.97	0.07	27,37,50,53	0
2	ANP	B	1001	31/31	0.97	0.06	26,34,49,56	0
2	ANP	A	1001	31/31	0.98	0.06	19,30,41,48	0
3	MG	C	1002	1/1	0.98	0.04	28,28,28,28	0
2	ANP	D	1001	31/31	0.98	0.06	27,34,42,50	0
3	MG	D	1002	1/1	0.99	0.05	25,25,25,25	0
3	MG	B	1002	1/1	1.00	0.04	32,32,32,32	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.

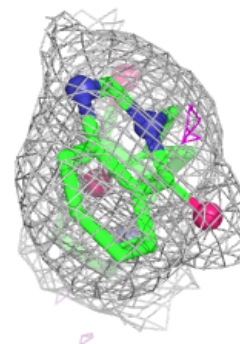
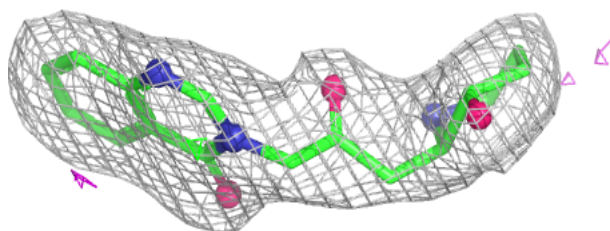
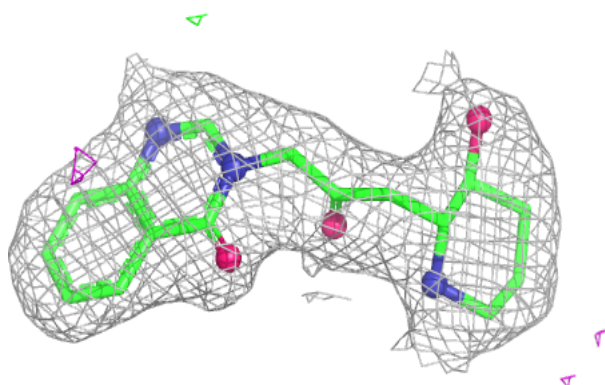


Electron density around 9SF C 1003:

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

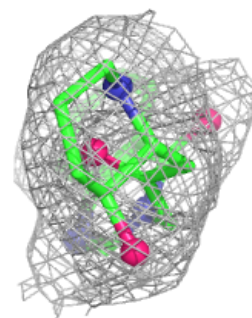
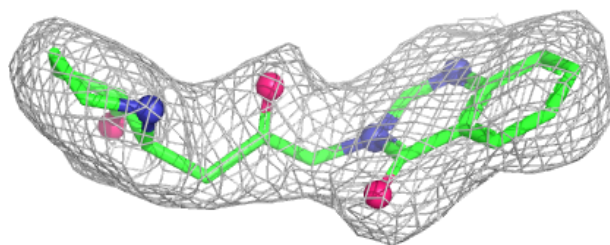
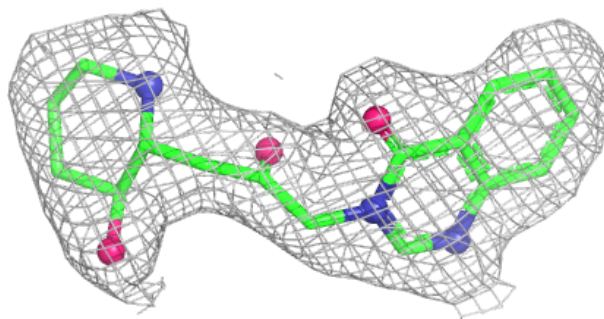
**Electron density around 9SF B 1003:**

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



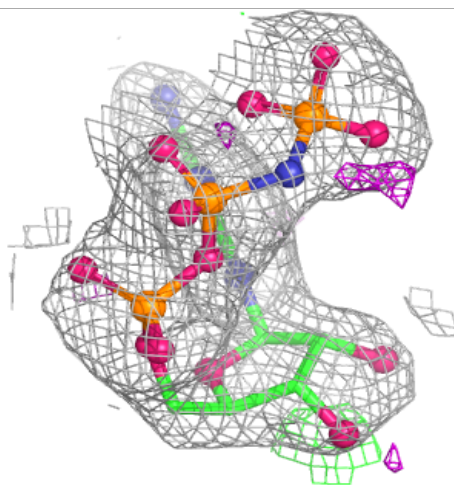
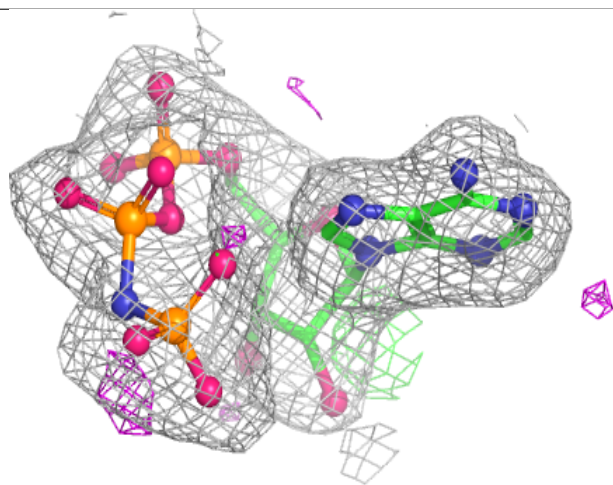
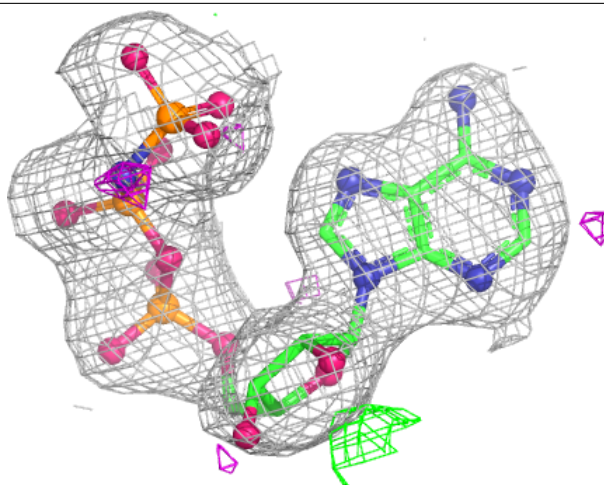
Electron density around 9SF D 1003:

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



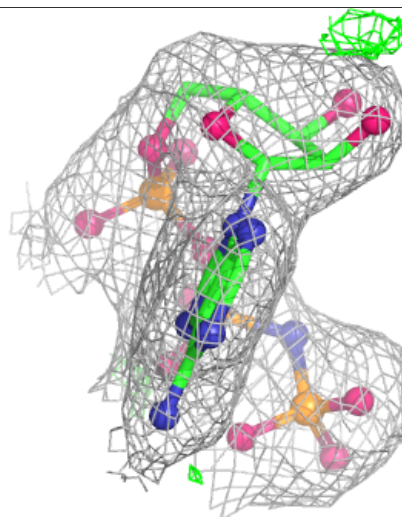
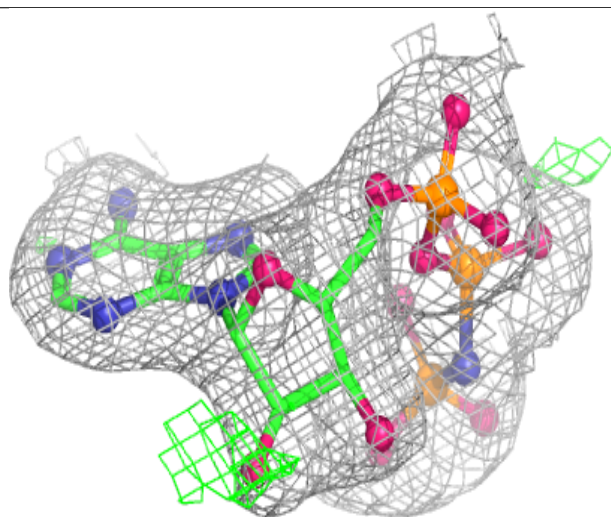
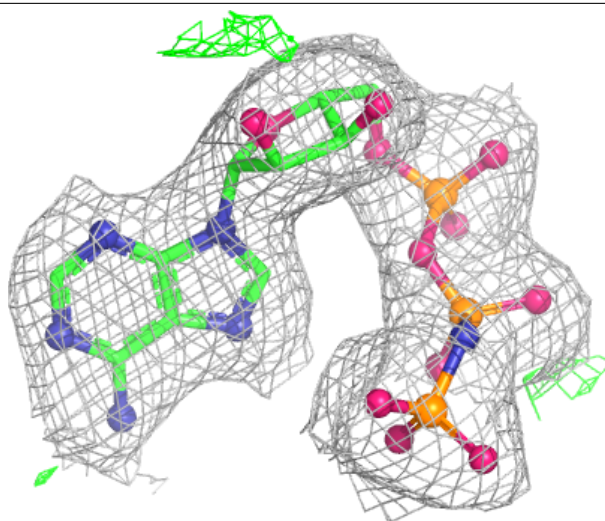
Electron density around ANP C 1001:

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



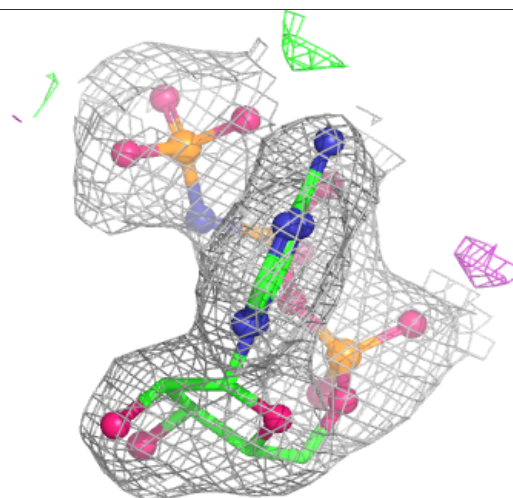
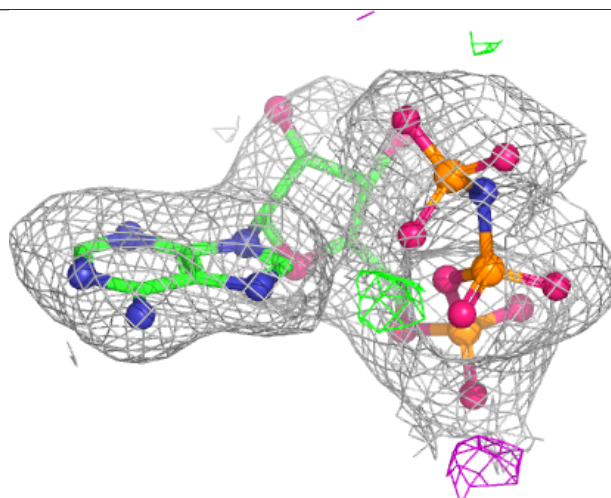
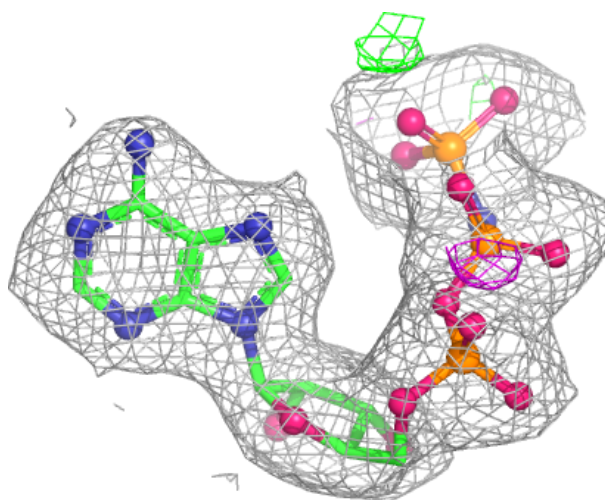
Electron density around ANP B 1001:

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



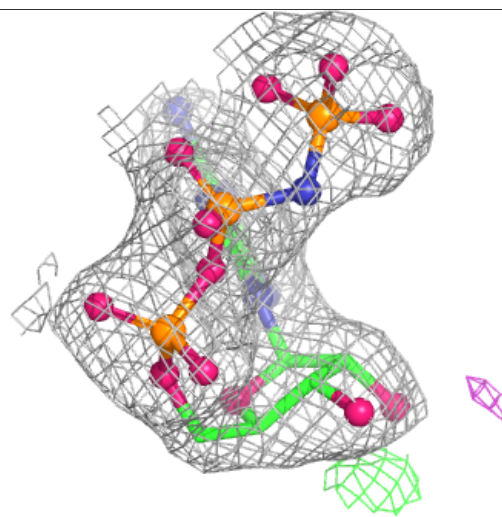
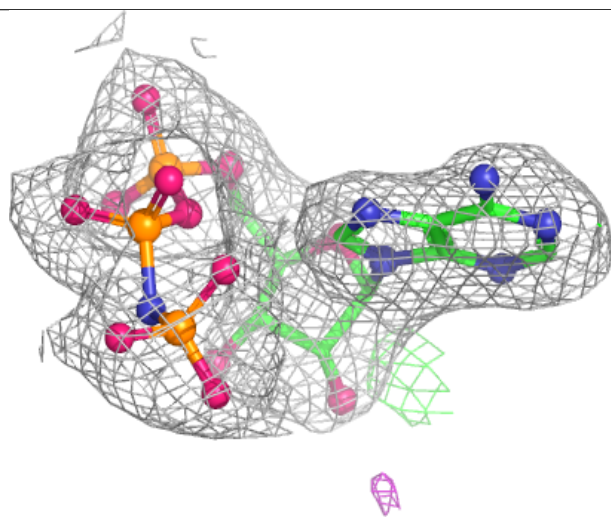
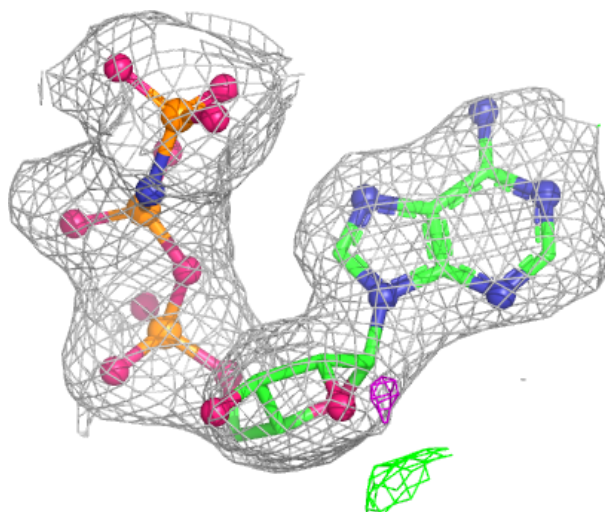
Electron density around ANP A 1001:

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



Electron density around ANP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.