



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:24 PM UTC

PDB ID : 4JZ7 / pdb_00004jz7
Title : Carbamate kinase from Giardia lamblia bound to AMP-PNP
Authors : Lim, K.; Herzberg, O.
Deposited on : 2013-04-02
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

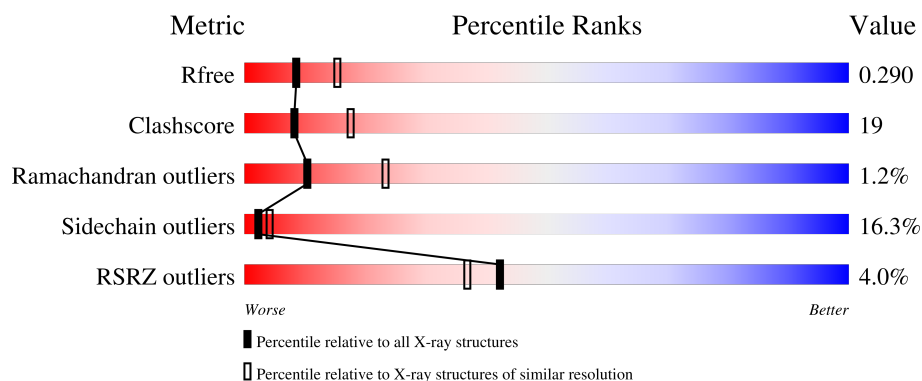
1 Overall quality at a glance

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	317	5% 55% 30% 5% 10%
1	B	317	2% 51% 32% 7% 10%
1	C	317	5% 57% 36% 7%
1	D	317	7% 54% 37% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9567 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.

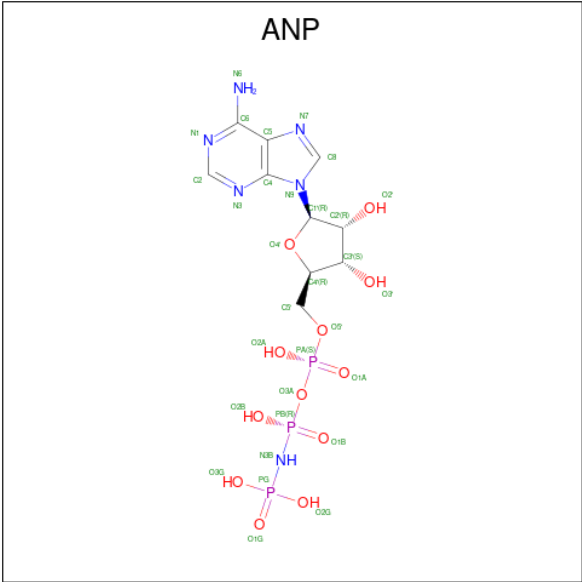
- Molecule 1 is a protein called Carbamate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2118	1329	360	411	18			
1	B	285	Total	C	N	O	S	0	0	0
			2118	1329	360	411	18			
1	C	316	Total	C	N	O	S	0	0	0
			2366	1483	408	456	19			
1	D	316	Total	C	N	O	S	0	0	0
			2366	1483	408	456	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	insertion	UNP A8BB85
B	0	GLY	-	insertion	UNP A8BB85
C	0	GLY	-	insertion	UNP A8BB85
D	0	GLY	-	insertion	UNP A8BB85

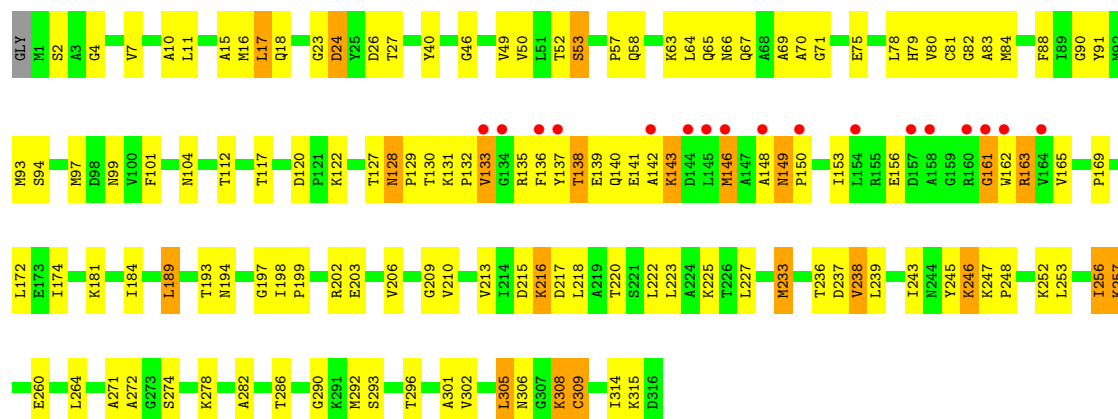
- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



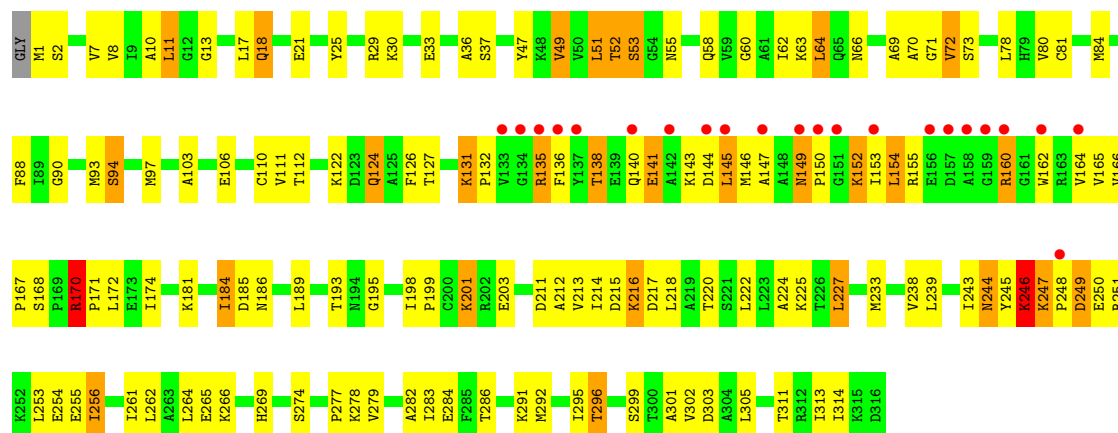
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	101	Total	O	0	0
			101	101		
3	C	119	Total	O	0	0
			119	119		
3	D	127	Total	O	0	0
			127	127		



● Molecule 1: Carbamate kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.63Å 97.05Å 102.12Å 90.00° 106.69° 90.00°	Depositor
Resolution (Å)	48.90 – 2.60 48.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (48.90-2.60) 99.3 (48.90-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.66 (at 2.61Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.217 , 0.292 0.211 , 0.290	Depositor DCC
R_{free} test set	1616 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9567	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5655e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62	0/2144	0.99	6/2898 (0.2%)
1	B	0.59	0/2144	0.93	1/2898 (0.0%)
1	C	0.64	0/2398	0.96	4/3240 (0.1%)
1	D	0.62	0/2398	1.01	6/3240 (0.2%)
All	All	0.62	0/9084	0.98	17/12276 (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	A	0	1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASN	CA-C-N	7.37	129.06	119.84
1	A	128	ASN	C-N-CA	7.37	129.06	119.84
1	D	152	LYS	N-CA-C	-7.30	98.82	110.14
1	D	131	LYS	CA-C-N	7.13	126.89	119.76
1	D	131	LYS	C-N-CA	7.13	126.89	119.76
1	C	272	ALA	N-CA-C	6.84	119.60	111.33
1	B	49	VAL	N-CA-C	6.21	116.80	108.11
1	D	170	ARG	CA-C-N	6.07	126.27	119.90
1	D	170	ARG	C-N-CA	6.07	126.27	119.90
1	C	15	ALA	N-CA-C	-5.99	105.80	113.23
1	D	49	VAL	N-CA-C	5.98	116.48	108.11
1	A	49	VAL	N-CA-C	5.89	116.36	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	146	MET	N-CA-C	-5.76	106.42	113.50
1	C	161	GLY	N-CA-C	5.40	117.47	110.45
1	A	166	VAL	CA-C-N	5.37	125.32	119.78
1	A	166	VAL	C-N-CA	5.37	125.32	119.78
1	A	52	THR	N-CA-C	-5.04	101.44	108.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	LYS	Peptide

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	2118	0	2186	73	0
1	B	2118	0	2186	87	0
1	C	2366	0	2430	92	0
1	D	2366	0	2430	113	0
2	A	31	0	13	1	0
2	B	31	0	13	6	0
2	C	31	0	13	5	0
2	D	31	0	13	4	0
3	A	128	0	0	5	0
3	B	101	0	0	9	0
3	C	119	0	0	6	0
3	D	127	0	0	14	0
All	All	9567	0	9284	354	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 19.

All (354) 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:C:216:LYS:HE2	1:C:217:ASP:OD1	1.59	1.01
1:B:67:GLN:HG3	1:B:75:GLU:OE1	1.71	0.91
1:A:243:ILE:HG21	1:A:264:LEU:HD13	1.57	0.87
1:B:131:LYS:O	1:B:166:VAL:HG22	1.77	0.84
1:A:315:LYS:HB2	3:A:1112:HOH:O	1.78	0.83
1:B:105:ASN:HB3	3:B:592:HOH:O	1.80	0.81
1:B:52:THR:HG21	1:B:220:THR:OG1	1.82	0.80
1:D:292:MET:HE2	1:D:314:ILE:HD11	1.64	0.79
1:A:164:VAL:HG12	1:A:165:VAL:H	1.47	0.78
1:A:225:LYS:HE2	3:A:1220:HOH:O	1.83	0.77
1:B:131:LYS:N	1:B:166:VAL:O	2.17	0.77
1:A:52:THR:HG21	1:A:220:THR:OG1	1.85	0.77
1:B:90:GLY:HA3	1:B:112:THR:HG21	1.67	0.77
1:D:52:THR:HG21	1:D:220:THR:OG1	1.85	0.76
1:B:255:GLU:C	1:B:256:ILE:HD13	2.10	0.76
1:C:136:PHE:HB3	1:C:161:GLY:HA3	1.67	0.76
1:B:258:LEU:HD21	1:B:287:GLN:HG2	1.70	0.73
1:C:52:THR:HG21	1:C:220:THR:OG1	1.89	0.72
1:C:127:THR:O	1:C:129:PRO:HD3	1.90	0.72
1:D:90:GLY:HA3	1:D:112:THR:HG21	1.72	0.71
1:D:256:ILE:HD11	1:D:311:THR:HG23	1.72	0.71
1:D:181:LYS:NZ	1:D:185:ASP:OD2	2.24	0.70
1:B:67:GLN:HB3	1:D:135:ARG:NH2	2.08	0.69
1:C:49:VAL:HB	1:C:189:LEU:HD13	1.75	0.69
1:C:90:GLY:HA3	1:C:112:THR:HG21	1.76	0.68
1:C:99:ASN:HA	3:C:509:HOH:O	1.94	0.68
1:D:154:LEU:HD12	1:D:162:TRP:HB3	1.75	0.67
1:C:156:GLU:HB2	1:C:162:TRP:CE2	2.30	0.67
1:D:216:LYS:HE2	1:D:217:ASP:OD1	1.95	0.67
1:B:216:LYS:HE2	1:B:217:ASP:OD1	1.95	0.66
1:A:129:PRO:CG	1:A:165:VAL:HG13	2.27	0.65
1:A:90:GLY:HA3	1:A:112:THR:HG21	1.79	0.65
1:B:72:VAL:O	1:D:160:ARG:NH2	2.25	0.64
1:C:236:THR:HG23	1:C:238:VAL:H	1.62	0.64
1:D:199:PRO:HG3	1:D:214:ILE:HG13	1.80	0.64
1:B:130:THR:N	1:B:166:VAL:O	2.29	0.64
1:C:82:GLY:HA3	3:C:525:HOH:O	1.98	0.64
1:C:138:THR:HG22	1:C:140:GLN:H	1.63	0.64
1:D:131:LYS:HE3	3:D:615:HOH:O	1.99	0.64
1:B:249:ASP:OD2	1:B:249:ASP:N	2.31	0.63
1:A:129:PRO:HG2	1:A:165:VAL:HG13	1.80	0.63
1:D:249:ASP:OD2	1:D:249:ASP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:MET:O	1:C:97:MET:HB2	1.99	0.62
1:D:69:ALA:C	1:D:71:GLY:H	2.06	0.62
1:A:66:ASN:O	1:A:75:GLU:HG3	1.99	0.62
1:B:243:ILE:HG22	1:B:269:HIS:CG	2.34	0.62
1:B:222:LEU:HA	1:B:225:LYS:HE2	1.82	0.62
1:A:245:TYR:CE2	1:A:246:LYS:HG2	2.35	0.62
1:A:234:ILE:HG21	1:A:278:LYS:HD3	1.81	0.61
1:C:49:VAL:HB	1:C:189:LEU:CD1	2.30	0.61
2:B:401:ANP:N3	2:B:401:ANP:H2'	2.14	0.61
1:C:84:MET:HB3	1:D:84:MET:HG2	1.83	0.61
1:D:55:ASN:ND2	1:D:195:GLY:HA3	2.16	0.61
1:C:215:ASP:HB3	1:C:218:LEU:HD12	1.82	0.61
1:B:22:LYS:O	1:B:24:ASP:N	2.30	0.60
1:B:75:GLU:OE2	1:D:141:GLU:OE2	2.19	0.60
1:A:308:LYS:O	1:A:309:CYS:HB3	1.99	0.60
1:D:292:MET:CE	1:D:314:ILE:HD11	2.32	0.60
1:D:69:ALA:O	1:D:71:GLY:N	2.34	0.60
1:D:201:LYS:HD3	3:D:518:HOH:O	2.02	0.59
1:B:236:THR:HG23	1:B:238:VAL:H	1.67	0.59
1:A:242:CYS:SG	1:A:252:LYS:HD3	2.42	0.59
1:A:79:HIS:HB3	1:A:210:VAL:O	2.01	0.59
1:C:247:LYS:HB3	1:C:248:PRO:HD2	1.84	0.59
1:D:261:ILE:HA	1:D:264:LEU:HB2	1.83	0.59
1:A:243:ILE:CG2	1:A:264:LEU:HD13	2.31	0.59
1:B:296:THR:HG23	1:B:310:GLY:HA3	1.84	0.59
1:C:278:LYS:NZ	2:C:401:ANP:O2B	2.33	0.59
1:B:40:TYR:OH	1:B:106:GLU:OE2	2.17	0.59
1:B:121:PRO:O	1:B:126:PHE:CD2	2.55	0.58
1:C:67:GLN:HG2	1:C:75:GLU:OE1	2.03	0.58
1:C:148:ALA:O	1:C:150:PRO:HD3	2.03	0.58
1:C:314:ILE:HG22	1:C:315:LYS:H	1.68	0.58
1:D:80:VAL:HG12	1:D:84:MET:HE2	1.85	0.58
1:B:278:LYS:NZ	2:B:401:ANP:O2B	2.32	0.58
1:D:244:ASN:ND2	1:D:249:ASP:O	2.36	0.58
1:B:263:ALA:O	1:B:266:LYS:HG3	2.03	0.58
1:C:292:MET:HG3	1:C:314:ILE:CD1	2.34	0.57
1:C:120:ASP:HB2	1:C:172:LEU:HD11	1.86	0.57
1:D:51:LEU:HD13	1:D:93:MET:HE2	1.85	0.57
1:D:78:LEU:N	1:D:211:ASP:OD2	2.35	0.57
1:B:69:ALA:C	1:B:71:GLY:H	2.13	0.57
1:D:149:ASN:OD1	1:D:149:ASN:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ASN:O	1:A:308:LYS:HE3	2.05	0.56
1:B:13:GLY:H	2:B:401:ANP:HNB1	1.51	0.56
1:D:153:ILE:O	1:D:164:VAL:HA	2.05	0.56
1:C:128:ASN:O	1:C:130:THR:HG23	2.04	0.56
1:D:243:ILE:HD11	1:D:251:ARG:HD3	1.87	0.56
1:D:282:ALA:HB1	1:D:313:ILE:HD12	1.88	0.56
1:B:282:ALA:HB1	1:B:313:ILE:HD12	1.87	0.56
1:C:292:MET:HG3	1:C:314:ILE:HD13	1.87	0.56
1:C:16:MET:O	1:C:17:LEU:HD13	2.07	0.55
1:D:295:ILE:O	1:D:296:THR:HG22	2.07	0.55
1:A:259:SER:HB3	1:A:316:ASP:OD2	2.07	0.55
1:B:97:MET:O	1:B:100:VAL:HG12	2.07	0.55
1:B:258:LEU:HD21	1:B:287:GLN:CG	2.37	0.55
1:B:279:VAL:HG12	1:B:283:ILE:HD12	1.89	0.55
1:D:244:ASN:HB3	1:D:247:LYS:HD2	1.89	0.55
1:C:80:VAL:HG13	1:D:88:PHE:CD1	2.42	0.55
1:D:49:VAL:HB	1:D:189:LEU:CD2	2.37	0.55
1:A:216:LYS:HE2	1:A:217:ASP:OD1	2.08	0.54
1:D:245:TYR:C	1:D:247:LYS:H	2.14	0.54
1:D:274:SER:O	1:D:277:PRO:HD2	2.08	0.54
1:A:239:LEU:HG	1:A:240:ASN:OD1	2.07	0.54
1:A:244:ASN:O	1:A:247:LYS:HB2	2.08	0.54
1:C:137:TYR:HB2	1:C:142:ALA:HB2	1.89	0.54
1:D:110:CYS:HB3	3:D:559:HOH:O	2.07	0.54
1:A:71:GLY:HA2	1:C:135:ARG:NH1	2.23	0.54
1:A:129:PRO:HB3	1:A:166:VAL:N	2.23	0.54
1:A:201:LYS:HD2	1:A:203:GLU:HG3	1.90	0.54
1:A:129:PRO:CB	1:A:165:VAL:HG13	2.37	0.54
1:B:170:ARG:NH1	1:B:284:GLU:OE1	2.41	0.54
1:D:154:LEU:HB3	1:D:162:TRP:HE3	1.73	0.54
1:B:246:LYS:N	1:B:250:GLU:OE1	2.33	0.53
1:C:181:LYS:O	1:C:184:ILE:HG13	2.07	0.53
1:A:164:VAL:HG12	1:A:165:VAL:N	2.22	0.53
1:C:52:THR:HG22	1:C:53:SER:N	2.22	0.53
1:C:133:VAL:HA	3:C:599:HOH:O	2.08	0.53
1:D:138:THR:HG22	1:D:141:GLU:CG	2.38	0.53
1:D:278:LYS:NZ	2:D:401:ANP:O2B	2.30	0.53
1:A:13:GLY:H	2:A:1001:ANP:HNB1	1.57	0.53
1:D:80:VAL:HG12	1:D:84:MET:CE	2.38	0.53
1:D:138:THR:HG22	1:D:141:GLU:HG2	1.89	0.53
1:D:238:VAL:HG21	2:D:401:ANP:H2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HG3	1:A:84:MET:HE1	1.91	0.53
1:A:262:LEU:HD23	1:A:283:ILE:HD13	1.91	0.53
1:C:256:ILE:HG13	1:C:260:GLU:OE2	2.09	0.53
1:D:256:ILE:CD1	1:D:311:THR:HG23	2.38	0.53
1:A:201:LYS:O	1:A:207:ILE:HA	2.09	0.53
1:A:216:LYS:NZ	3:A:1104:HOH:O	2.40	0.53
1:B:8:VAL:HG21	1:B:224:ALA:HA	1.90	0.53
1:D:29:ARG:HH21	1:D:30:LYS:HB3	1.74	0.53
1:B:239:LEU:HD12	1:B:297:SER:HB3	1.91	0.52
1:C:26:ASP:HB2	3:C:566:HOH:O	2.08	0.52
1:C:131:LYS:HD2	1:C:132:PRO:HD2	1.92	0.52
1:D:215:ASP:HB3	1:D:218:LEU:HD12	1.92	0.52
1:C:314:ILE:HG22	1:C:315:LYS:N	2.23	0.52
1:D:145:LEU:HD22	1:D:149:ASN:OD1	2.10	0.52
1:D:174:ILE:HD12	1:D:222:LEU:HD23	1.91	0.52
1:D:135:ARG:HG2	1:D:136:PHE:N	2.24	0.51
1:A:234:ILE:CG2	1:A:278:LYS:HD3	2.40	0.51
1:A:296:THR:HG23	1:A:310:GLY:HA3	1.92	0.51
1:B:88:PHE:CD1	1:B:88:PHE:C	2.88	0.51
1:C:52:THR:CG2	1:C:53:SER:N	2.74	0.51
1:A:131:LYS:HG3	1:A:132:PRO:HD2	1.91	0.51
1:B:14:ASN:HA	1:B:17:LEU:O	2.11	0.51
1:D:233:MET:HE1	1:D:301:ALA:O	2.10	0.51
1:C:138:THR:CG2	1:C:139:GLU:N	2.73	0.51
1:C:233:MET:HE1	1:C:301:ALA:O	2.11	0.51
1:A:300:THR:O	1:A:300:THR:OG1	2.24	0.51
1:C:237:ASP:OD1	2:C:401:ANP:O3'	2.25	0.51
1:C:222:LEU:HA	1:C:225:LYS:HZ1	1.75	0.50
1:C:65:GLN:NE2	1:D:66:ASN:OD1	2.45	0.50
1:D:170:ARG:NH1	1:D:284:GLU:OE1	2.45	0.50
1:A:215:ASP:HB3	1:A:218:LEU:HD12	1.94	0.50
1:B:263:ALA:HA	1:B:266:LYS:HE3	1.94	0.50
1:B:67:GLN:CG	1:B:75:GLU:OE1	2.53	0.50
1:A:296:THR:HG23	1:A:310:GLY:CA	2.42	0.50
1:B:201:LYS:NZ	1:B:208:SER:OG	2.28	0.50
1:B:239:LEU:HB3	1:B:240:ASN:OD1	2.12	0.50
1:C:128:ASN:N	1:C:128:ASN:OD1	2.45	0.50
1:C:282:ALA:HB1	1:C:293:SER:HB3	1.93	0.50
1:A:83:ALA:HA	1:A:198:ILE:HD11	1.94	0.49
1:C:83:ALA:HA	1:C:198:ILE:HD11	1.95	0.49
1:D:53:SER:O	1:D:216:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:286:THR:HG23	1:D:291:LYS:O	2.13	0.49
1:A:181:LYS:HD3	1:A:185:ASP:OD2	2.13	0.49
1:C:194:ASN:ND2	3:C:571:HOH:O	2.34	0.49
1:B:233:MET:HE1	1:B:301:ALA:O	2.12	0.48
1:B:274:SER:HB2	2:B:401:ANP:O4'	2.13	0.48
2:D:401:ANP:N7	3:D:555:HOH:O	2.34	0.48
1:B:51:LEU:HD13	1:B:93:MET:HE2	1.95	0.48
1:D:295:ILE:C	1:D:296:THR:CG2	2.86	0.48
1:B:52:THR:CG2	1:B:53:SER:N	2.75	0.48
1:C:53:SER:OG	1:C:93:MET:HE1	2.12	0.48
1:D:52:THR:CG2	1:D:53:SER:N	2.77	0.48
1:B:110:CYS:SG	1:B:111:VAL:N	2.86	0.48
1:B:121:PRO:HA	1:B:126:PHE:CE2	2.48	0.48
1:D:253:LEU:HB3	1:D:256:ILE:HD11	1.96	0.48
1:A:166:VAL:HG23	1:A:212:ALA:HA	1.95	0.48
1:D:69:ALA:C	1:D:71:GLY:N	2.71	0.48
1:A:18:GLN:HB2	1:A:21:GLU:OE2	2.14	0.48
1:A:248:PRO:C	1:A:250:GLU:H	2.21	0.48
1:C:91:TYR:CE1	1:D:198:ILE:HG21	2.48	0.48
1:C:169:PRO:HD2	1:C:213:VAL:O	2.13	0.48
1:C:216:LYS:NZ	2:C:401:ANP:O2G	2.44	0.48
1:A:53:SER:O	1:A:216:LYS:HG3	2.13	0.48
1:D:64:LEU:O	1:D:64:LEU:HD22	2.14	0.48
1:B:16:MET:O	1:B:17:LEU:HD13	2.14	0.48
1:C:58:GLN:H	1:C:58:GLN:CD	2.21	0.48
1:D:18:GLN:O	1:D:21:GLU:HB2	2.14	0.48
1:B:201:LYS:HE2	3:B:555:HOH:O	2.14	0.47
1:B:263:ALA:HA	1:B:266:LYS:HG2	1.95	0.47
1:C:222:LEU:HA	1:C:225:LYS:NZ	2.29	0.47
1:A:78:LEU:HD23	1:A:212:ALA:N	2.29	0.47
1:A:130:THR:HG22	1:A:131:LYS:N	2.28	0.47
1:B:180:ILE:O	1:B:184:ILE:HG12	2.14	0.47
1:D:147:ALA:O	1:D:150:PRO:HG3	2.14	0.47
1:A:63:LYS:HD2	1:A:63:LYS:HA	1.63	0.47
1:C:24:ASP:OD2	1:C:27:THR:N	2.34	0.47
1:D:184:ILE:HD11	3:D:611:HOH:O	2.14	0.47
1:C:308:LYS:O	1:C:309:CYS:HB3	2.13	0.47
1:D:49:VAL:HB	1:D:189:LEU:HD21	1.95	0.47
1:D:189:LEU:HD13	1:D:189:LEU:C	2.40	0.47
1:A:53:SER:C	1:A:216:LYS:HG3	2.39	0.47
1:C:243:ILE:HG21	1:C:264:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:O	1:D:62:ILE:HG12	2.15	0.47
1:C:129:PRO:O	1:C:165:VAL:HB	2.14	0.47
1:B:307:GLY:HA2	3:B:554:HOH:O	2.15	0.47
2:B:401:ANP:O1G	3:B:549:HOH:O	2.21	0.47
1:C:91:TYR:CD1	1:D:198:ILE:HD13	2.50	0.47
1:C:306:ASN:O	1:C:308:LYS:HD3	2.15	0.46
1:D:254:GLU:OE1	1:D:254:GLU:HA	2.14	0.46
1:C:88:PHE:CD1	1:D:80:VAL:HG13	2.50	0.46
1:B:107:PRO:HG2	3:B:590:HOH:O	2.16	0.46
1:C:50:VAL:HG11	1:C:223:LEU:HD21	1.98	0.46
1:C:117:THR:OG1	1:C:197:GLY:HA3	2.15	0.46
1:C:286:THR:O	1:C:290:GLY:N	2.44	0.46
1:D:90:GLY:O	1:D:94:SER:HB2	2.16	0.46
1:C:10:ALA:HB2	1:C:220:THR:HG21	1.98	0.46
1:C:149:ASN:OD1	1:C:149:ASN:N	2.48	0.46
1:B:86:GLN:HG2	1:B:194:ASN:HB2	1.97	0.46
1:D:255:GLU:C	1:D:256:ILE:HG13	2.40	0.46
1:A:120:ASP:HB2	1:A:172:LEU:HD11	1.98	0.46
1:B:69:ALA:O	1:B:71:GLY:N	2.49	0.46
1:D:126:PHE:CD1	1:D:167:PRO:HG2	2.50	0.46
1:D:244:ASN:HB3	1:D:247:LYS:CD	2.46	0.46
2:C:401:ANP:H2'	2:C:401:ANP:N3	2.30	0.46
1:D:1:MET:HE1	1:D:47:TYR:O	2.16	0.46
1:D:51:LEU:HD23	1:D:51:LEU:HA	1.59	0.46
1:B:300:THR:HG22	3:B:563:HOH:O	2.15	0.46
1:D:143:LYS:HA	1:D:146:MET:HE2	1.98	0.46
1:A:118:LEU:HD23	1:A:200:CYS:HB2	1.97	0.46
1:A:278:LYS:O	1:A:281:ALA:HB3	2.15	0.46
1:B:69:ALA:HB1	1:B:72:VAL:HG23	1.97	0.46
1:C:69:ALA:C	1:C:71:GLY:H	2.24	0.46
1:A:249:ASP:OD2	1:A:249:ASP:N	2.49	0.45
1:D:58:GLN:HA	3:D:550:HOH:O	2.15	0.45
1:D:60:GLY:HA2	3:D:569:HOH:O	2.15	0.45
1:A:18:GLN:HB2	1:A:21:GLU:CD	2.42	0.45
1:D:170:ARG:HA	1:D:171:PRO:HD3	1.79	0.45
1:B:88:PHE:O	1:B:91:TYR:HB3	2.17	0.45
1:B:309:CYS:O	1:B:312:ARG:NE	2.50	0.45
1:A:204:ASN:O	1:A:205:LYS:HB2	2.16	0.45
1:B:11:LEU:O	1:B:216:LYS:HE3	2.16	0.45
1:D:299:SER:HB3	3:D:521:HOH:O	2.17	0.45
1:A:239:LEU:HA	1:A:297:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:LYS:HG3	1:C:133:VAL:HG23	1.99	0.45
1:C:156:GLU:HG2	1:C:161:GLY:O	2.16	0.45
1:D:245:TYR:O	1:D:247:LYS:N	2.50	0.45
1:C:225:LYS:NZ	3:C:504:HOH:O	2.48	0.45
1:A:200:CYS:HB3	1:A:207:ILE:HG23	1.99	0.45
1:B:69:ALA:C	1:B:71:GLY:N	2.75	0.45
1:B:244:ASN:HA	1:B:247:LYS:NZ	2.32	0.45
1:C:57:PRO:HG2	1:C:58:GLN:OE1	2.17	0.45
1:B:129:PRO:O	1:B:130:THR:HG23	2.17	0.44
1:C:80:VAL:HG21	1:D:25:TYR:CD1	2.52	0.44
1:C:292:MET:HE2	1:C:314:ILE:HD11	1.99	0.44
1:D:8:VAL:HG21	1:D:224:ALA:HA	2.00	0.44
1:C:79:HIS:CE1	1:C:209:GLY:HA3	2.52	0.44
1:C:271:ALA:HB3	1:C:274:SER:OG	2.17	0.44
1:B:130:THR:C	1:B:165:VAL:HG22	2.43	0.44
1:C:246:LYS:HD2	1:C:246:LYS:HA	1.62	0.44
1:D:303:ASP:HA	3:D:510:HOH:O	2.18	0.44
1:B:254:GLU:N	1:B:256:ILE:HD11	2.32	0.44
1:D:36:ALA:HA	1:D:97:MET:HE1	2.00	0.44
1:A:32:VAL:O	1:A:36:ALA:N	2.50	0.44
1:B:79:HIS:HB3	1:B:210:VAL:O	2.18	0.44
1:D:131:LYS:HA	1:D:132:PRO:HD3	1.65	0.44
1:C:4:GLY:HA3	1:C:46:GLY:O	2.18	0.44
1:C:202:ARG:HA	1:C:206:VAL:O	2.18	0.44
1:D:199:PRO:HG2	1:D:212:ALA:O	2.17	0.44
1:C:18:GLN:HA	1:C:18:GLN:OE1	2.18	0.44
1:B:208:SER:HB3	3:B:555:HOH:O	2.18	0.43
1:C:129:PRO:HB2	1:C:165:VAL:O	2.18	0.43
1:A:308:LYS:HA	1:A:308:LYS:HD3	1.83	0.43
1:A:316:ASP:HA	3:A:1131:HOH:O	2.19	0.43
1:D:245:TYR:C	1:D:247:LYS:N	2.76	0.43
1:D:262:LEU:HD23	1:D:262:LEU:HA	1.74	0.43
1:D:10:ALA:HB2	1:D:220:THR:HG21	2.01	0.43
1:C:78:LEU:O	1:C:81:CYS:HB2	2.19	0.43
1:C:136:PHE:CE2	1:C:163:ARG:HD3	2.54	0.43
1:D:295:ILE:C	1:D:296:THR:HG22	2.44	0.43
1:B:242:CYS:SG	1:B:252:LYS:HG3	2.59	0.43
1:C:52:THR:CG2	1:C:53:SER:H	2.31	0.43
1:D:1:MET:HE2	1:D:1:MET:HB3	1.95	0.43
1:D:124:GLN:H	1:D:124:GLN:HG3	1.63	0.43
1:D:246:LYS:HD2	1:D:246:LYS:HA	1.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD11	1:B:84:MET:HE2	2.00	0.43
1:A:78:LEU:HB3	1:A:211:ASP:OD2	2.19	0.43
1:B:93:MET:O	1:B:97:MET:HB2	2.19	0.43
1:D:243:ILE:HG21	1:D:264:LEU:HD13	2.01	0.43
1:A:171:PRO:HG3	1:A:214:ILE:CG2	2.49	0.42
1:C:101:PHE:CZ	1:C:189:LEU:HD23	2.54	0.42
1:D:243:ILE:HB	1:D:269:HIS:ND1	2.33	0.42
1:C:63:LYS:HG2	1:C:133:VAL:HG13	2.01	0.42
1:D:81:CYS:HA	1:D:84:MET:HE3	2.01	0.42
1:D:166:VAL:HA	1:D:167:PRO:HD3	1.86	0.42
1:C:245:TYR:O	1:C:246:LYS:HB2	2.18	0.42
1:A:87:GLY:HA3	1:B:83:ALA:O	2.20	0.42
1:C:120:ASP:OD1	1:C:122:LYS:N	2.52	0.42
1:D:18:GLN:NE2	3:D:534:HOH:O	2.52	0.42
1:D:170:ARG:HG3	1:D:171:PRO:HD2	2.02	0.42
1:D:247:LYS:NZ	3:D:573:HOH:O	2.31	0.42
1:B:17:LEU:HD13	1:B:28:GLN:HG2	2.01	0.42
1:B:247:LYS:HG2	1:B:248:PRO:HD2	2.00	0.42
1:A:62:ILE:HD13	1:A:84:MET:HB2	2.00	0.42
1:B:64:LEU:O	1:B:64:LEU:HD22	2.20	0.42
1:B:274:SER:OG	2:B:401:ANP:H8	2.19	0.42
1:D:18:GLN:HB2	1:D:21:GLU:OE2	2.18	0.42
1:B:170:ARG:NH1	1:B:284:GLU:OE2	2.52	0.42
1:B:312:ARG:HD2	3:B:554:HOH:O	2.20	0.42
1:C:239:LEU:HD12	1:C:239:LEU:O	2.19	0.42
1:C:282:ALA:HB1	1:C:293:SER:CB	2.50	0.42
1:A:33:GLU:HG2	3:A:1169:HOH:O	2.18	0.42
1:D:13:GLY:H	2:D:401:ANP:HNB1	1.66	0.42
1:D:78:LEU:HD23	1:D:212:ALA:N	2.35	0.42
1:C:305:LEU:HD12	1:C:305:LEU:HA	1.92	0.42
1:A:222:LEU:HA	1:A:225:LYS:HE3	2.01	0.42
1:B:263:ALA:HA	1:B:266:LYS:CG	2.50	0.42
1:C:40:TYR:CE2	1:C:104:ASN:CG	2.98	0.42
1:D:168:SER:HA	1:D:213:VAL:O	2.20	0.42
1:D:189:LEU:HD22	1:D:189:LEU:HA	1.85	0.42
1:B:166:VAL:HB	1:B:167:PRO:CD	2.50	0.41
1:C:278:LYS:CE	2:C:401:ANP:O2B	2.68	0.41
1:A:11:LEU:O	1:A:216:LYS:HE3	2.21	0.41
1:A:84:MET:HG2	1:B:88:PHE:HB2	2.01	0.41
1:B:55:ASN:CG	1:B:195:GLY:HA3	2.45	0.41
1:B:1:MET:HE2	1:B:1:MET:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LEU:HA	1:B:264:LEU:HD23	1.80	0.41
1:D:247:LYS:O	1:D:249:ASP:N	2.52	0.41
1:A:84:MET:HB3	1:B:84:MET:HB3	2.02	0.41
1:D:11:LEU:HD12	1:D:11:LEU:HA	1.91	0.41
1:D:243:ILE:CG2	1:D:264:LEU:HD13	2.51	0.41
1:A:244:ASN:HB2	1:A:250:GLU:HA	2.02	0.41
1:B:62:ILE:HG22	1:B:81:CYS:SG	2.61	0.41
1:C:198:ILE:HA	1:C:199:PRO:HD3	1.96	0.41
1:D:69:ALA:HB1	1:D:72:VAL:HG23	2.02	0.41
1:D:246:LYS:H	1:D:250:GLU:CD	2.29	0.41
1:A:97:MET:O	1:A:101:PHE:HD1	2.03	0.41
1:D:186:ASN:ND2	3:D:529:HOH:O	2.31	0.41
1:A:198:ILE:HA	1:A:199:PRO:HD3	1.94	0.40
1:D:225:LYS:NZ	3:D:538:HOH:O	2.54	0.40
1:B:243:ILE:HG22	1:B:269:HIS:CB	2.51	0.40
1:A:110:CYS:HB2	1:A:189:LEU:O	2.22	0.40
1:A:258:LEU:HD22	1:A:286:THR:HG22	2.03	0.40
1:B:170:ARG:NH1	1:B:284:GLU:CD	2.80	0.40
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.86	0.40
1:A:91:TYR:O	1:A:94:SER:HB2	2.21	0.40
1:B:110:CYS:HB3	3:B:541:HOH:O	2.21	0.40
1:B:170:ARG:NH2	1:B:218:LEU:HD13	2.36	0.40
1:C:256:ILE:HG12	1:C:257:LYS:N	2.36	0.40
1:D:103:ALA:HB2	3:D:583:HOH:O	2.22	0.40
1:C:143:LYS:O	1:C:143:LYS:HG2	2.21	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	281/317 (89%)	253 (90%)	24 (8%)	4 (1%)	9 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	281/317 (89%)	265 (94%)	13 (5%)	3 (1%)	11	25
1	C	314/317 (99%)	292 (93%)	19 (6%)	3 (1%)	12	28
1	D	314/317 (99%)	283 (90%)	27 (9%)	4 (1%)	9	21
All	All	1190/1268 (94%)	1093 (92%)	83 (7%)	14 (1%)	10	23

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	PRO
1	B	70	ALA
1	D	70	ALA
1	A	309	CYS
1	B	23	GLY
1	D	160	ARG
1	A	248	PRO
1	C	70	ALA
1	A	249	ASP
1	B	130	THR
1	C	309	CYS
1	D	246	LYS
1	D	248	PRO
1	C	23	GLY

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	234/257 (91%)	203 (87%)	31 (13%)	4	8
1	B	234/257 (91%)	193 (82%)	41 (18%)	2	3
1	C	257/257 (100%)	221 (86%)	36 (14%)	3	6
1	D	257/257 (100%)	205 (80%)	52 (20%)	1	2
All	All	982/1028 (96%)	822 (84%)	160 (16%)	2	4

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	VAL
1	A	11	LEU
1	A	17	LEU
1	A	18	GLN
1	A	30	LYS
1	A	37	SER
1	A	48	LYS
1	A	64	LEU
1	A	122	LYS
1	A	124	GLN
1	A	131	LYS
1	A	165	VAL
1	A	166	VAL
1	A	174	ILE
1	A	184	ILE
1	A	187	ASN
1	A	193	THR
1	A	210	VAL
1	A	216	LYS
1	A	221	SER
1	A	227	LEU
1	A	239	LEU
1	A	247	LYS
1	A	250	GLU
1	A	256	ILE
1	A	257	LYS
1	A	261	ILE
1	A	266	LYS
1	A	284	GLU
1	A	296	THR
1	B	2	SER
1	B	7	VAL
1	B	11	LEU
1	B	17	LEU
1	B	20	LYS
1	B	22	LYS
1	B	29	ARG
1	B	52	THR
1	B	59	VAL
1	B	63	LYS
1	B	64	LEU

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Mol	Chain	Res	Type
1	B	72	VAL
1	B	73	SER
1	B	110	CYS
1	B	111	VAL
1	B	122	LYS
1	B	127	THR
1	B	130	THR
1	B	165	VAL
1	B	168	SER
1	B	184	ILE
1	B	189	LEU
1	B	193	THR
1	B	201	LYS
1	B	203	GLU
1	B	208	SER
1	B	216	LYS
1	B	227	LEU
1	B	239	LEU
1	B	243	ILE
1	B	246	LYS
1	B	247	LYS
1	B	252	LYS
1	B	253	LEU
1	B	256	ILE
1	B	261	ILE
1	B	266	LYS
1	B	292	MET
1	B	295	ILE
1	B	296	THR
1	B	305	LEU
1	C	2	SER
1	C	7	VAL
1	C	11	LEU
1	C	17	LEU
1	C	24	ASP
1	C	53	SER
1	C	64	LEU
1	C	66	ASN
1	C	94	SER
1	C	128	ASN
1	C	133	VAL
1	C	138	THR

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Mol	Chain	Res	Type
1	C	141	GLU
1	C	143	LYS
1	C	146	MET
1	C	149	ASN
1	C	153	ILE
1	C	163	ARG
1	C	174	ILE
1	C	189	LEU
1	C	193	THR
1	C	203	GLU
1	C	210	VAL
1	C	216	LYS
1	C	227	LEU
1	C	233	MET
1	C	238	VAL
1	C	246	LYS
1	C	252	LYS
1	C	253	LEU
1	C	256	ILE
1	C	257	LYS
1	C	296	THR
1	C	302	VAL
1	C	305	LEU
1	C	308	LYS
1	D	2	SER
1	D	7	VAL
1	D	11	LEU
1	D	17	LEU
1	D	18	GLN
1	D	33	GLU
1	D	37	SER
1	D	51	LEU
1	D	52	THR
1	D	53	SER
1	D	63	LYS
1	D	64	LEU
1	D	72	VAL
1	D	73	SER
1	D	94	SER
1	D	106	GLU
1	D	111	VAL
1	D	122	LYS

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Mol	Chain	Res	Type
1	D	124	GLN
1	D	127	THR
1	D	135	ARG
1	D	138	THR
1	D	140	GLN
1	D	141	GLU
1	D	144	ASP
1	D	145	LEU
1	D	149	ASN
1	D	152	LYS
1	D	154	LEU
1	D	155	ARG
1	D	165	VAL
1	D	170	ARG
1	D	172	LEU
1	D	184	ILE
1	D	193	THR
1	D	201	LYS
1	D	203	GLU
1	D	216	LYS
1	D	227	LEU
1	D	239	LEU
1	D	244	ASN
1	D	246	LYS
1	D	247	LYS
1	D	249	ASP
1	D	256	ILE
1	D	265	GLU
1	D	266	LYS
1	D	279	VAL
1	D	283	ILE
1	D	296	THR
1	D	302	VAL
1	D	305	LEU

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	228	ASN
1	A	269	HIS
1	B	95	GLN
1	B	104	ASN

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Mol	Chain	Res	Type
1	B	128	ASN
1	B	287	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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
2	ANP	D	401	-	33,33,33	2.05	5 (15%)	45,52,52	1.97	12 (26%)
2	ANP	A	1001	-	33,33,33	1.99	6 (18%)	45,52,52	1.98	14 (31%)
2	ANP	C	401	-	33,33,33	2.20	8 (24%)	45,52,52	1.98	15 (33%)
2	ANP	B	401	-	33,33,33	1.98	5 (15%)	45,52,52	1.97	12 (26%)

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
2	ANP	D	401	-	-	7/18/38/38	0/3/3/3
2	ANP	A	1001	-	-	8/18/38/38	0/3/3/3
2	ANP	C	401	-	-	6/18/38/38	0/3/3/3
2	ANP	B	401	-	-	5/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	ANP	PB-O1B	6.58	1.56	1.46
2	D	401	ANP	PB-O1B	6.14	1.55	1.46
2	A	1001	ANP	PB-O1B	6.09	1.55	1.46
2	B	401	ANP	PB-O1B	5.63	1.54	1.46
2	B	401	ANP	C6-N6	5.37	1.47	1.34
2	C	401	ANP	C6-N6	5.30	1.47	1.34
2	D	401	ANP	C6-N6	5.25	1.47	1.34
2	A	1001	ANP	C6-N6	5.08	1.47	1.34
2	C	401	ANP	PG-O1G	4.01	1.52	1.46
2	D	401	ANP	PG-O1G	3.67	1.51	1.46
2	D	401	ANP	O4'-C4'	-3.61	1.37	1.45
2	B	401	ANP	PG-O1G	3.56	1.51	1.46
2	A	1001	ANP	PG-O1G	3.40	1.51	1.46
2	A	1001	ANP	C2'-C3'	-3.35	1.44	1.53
2	B	401	ANP	O4'-C4'	-3.28	1.37	1.45
2	C	401	ANP	C2'-C3'	-3.26	1.44	1.53
2	A	1001	ANP	O4'-C4'	-3.26	1.37	1.45
2	B	401	ANP	C2'-C3'	-3.17	1.44	1.53
2	D	401	ANP	C2'-C3'	-3.10	1.45	1.53
2	C	401	ANP	PB-O3A	-3.09	1.55	1.59
2	C	401	ANP	O4'-C4'	-2.97	1.38	1.45
2	C	401	ANP	PB-N3B	2.15	1.69	1.63
2	A	1001	ANP	C2'-C1'	-2.11	1.46	1.53
2	C	401	ANP	C2'-C1'	-2.07	1.47	1.53

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	ANP	N3-C2-N1	-5.38	120.43	128.58
2	B	401	ANP	N3-C2-N1	-5.36	120.46	128.58
2	D	401	ANP	N3-C2-N1	-5.04	120.96	128.58
2	C	401	ANP	N3-C2-N1	-5.03	120.97	128.58
2	C	401	ANP	C5-C4-N3	-4.87	120.02	126.72
2	A	1001	ANP	C5-C4-N3	-4.63	120.34	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ANP	C5-C4-N3	-4.45	120.59	126.72
2	C	401	ANP	N3-C4-N9	4.23	134.36	127.17
2	D	401	ANP	C4-N9-C8	4.15	110.09	105.74
2	D	401	ANP	C5-C4-N3	-4.09	121.08	126.72
2	B	401	ANP	N9-C8-N7	-4.08	108.15	113.94
2	D	401	ANP	N9-C8-N7	-4.04	108.20	113.94
2	A	1001	ANP	N3-C4-N9	3.98	133.93	127.17
2	B	401	ANP	N3-C4-N9	3.87	133.75	127.17
2	B	401	ANP	C4-N9-C8	3.87	109.80	105.74
2	D	401	ANP	N3-C4-N9	3.61	133.30	127.17
2	C	401	ANP	C4-N9-C8	3.54	109.45	105.74
2	C	401	ANP	N9-C8-N7	-3.50	108.96	113.94
2	A	1001	ANP	N9-C8-N7	-3.50	108.97	113.94
2	A	1001	ANP	C4-N9-C8	3.45	109.36	105.74
2	A	1001	ANP	C2-N3-C4	3.42	120.18	111.83
2	D	401	ANP	C5-N7-C8	3.31	108.65	103.45
2	C	401	ANP	C2-N3-C4	3.30	119.90	111.83
2	B	401	ANP	C2-N3-C4	3.27	119.81	111.83
2	B	401	ANP	C5-N7-C8	3.26	108.58	103.45
2	C	401	ANP	O5'-C5'-C4'	3.23	120.00	108.99
2	A	1001	ANP	O3A-PB-N3B	3.21	115.50	106.59
2	D	401	ANP	C2'-C1'-N9	3.08	120.97	113.30
2	C	401	ANP	C5-N7-C8	3.04	108.23	103.45
2	C	401	ANP	O3A-PB-N3B	3.01	114.94	106.59
2	D	401	ANP	C2-N3-C4	2.98	119.11	111.83
2	A	1001	ANP	C5-N7-C8	2.91	108.02	103.45
2	D	401	ANP	O4'-C1'-N9	-2.82	102.67	108.09
2	A	1001	ANP	C3'-C2'-C1'	2.77	106.71	101.46
2	D	401	ANP	C4-C5-N7	-2.76	107.43	110.58
2	B	401	ANP	O3A-PB-N3B	2.69	114.05	106.59
2	A	1001	ANP	C2'-C1'-N9	2.69	119.98	113.30
2	B	401	ANP	C3'-C2'-C1'	2.65	106.48	101.46
2	C	401	ANP	C4-C5-N7	-2.50	107.72	110.58
2	B	401	ANP	C2-N1-C6	2.49	122.82	118.73
2	A	1001	ANP	C2-N1-C6	2.45	122.75	118.73
2	D	401	ANP	C3'-C2'-C1'	2.43	106.06	101.46
2	D	401	ANP	C2-N1-C6	2.42	122.71	118.73
2	B	401	ANP	C4-C5-N7	-2.42	107.81	110.58
2	A	1001	ANP	C4-C5-N7	-2.33	107.92	110.58
2	C	401	ANP	C2-N1-C6	2.32	122.54	118.73
2	C	401	ANP	C3'-C2'-C1'	2.31	105.83	101.46
2	C	401	ANP	C2'-C1'-N9	2.25	118.90	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	ANP	O5'-C5'-C4'	2.18	116.41	108.99
2	A	1001	ANP	O5'-C5'-C4'	2.08	116.08	108.99
2	C	401	ANP	O2G-PG-O1G	-2.07	108.27	113.45
2	C	401	ANP	O3G-PG-O1G	-2.02	108.38	113.45
2	A	1001	ANP	O2G-PG-O1G	-2.01	108.40	113.45

There are no chirality outliers.

All (26) torsion outliers are listed below:

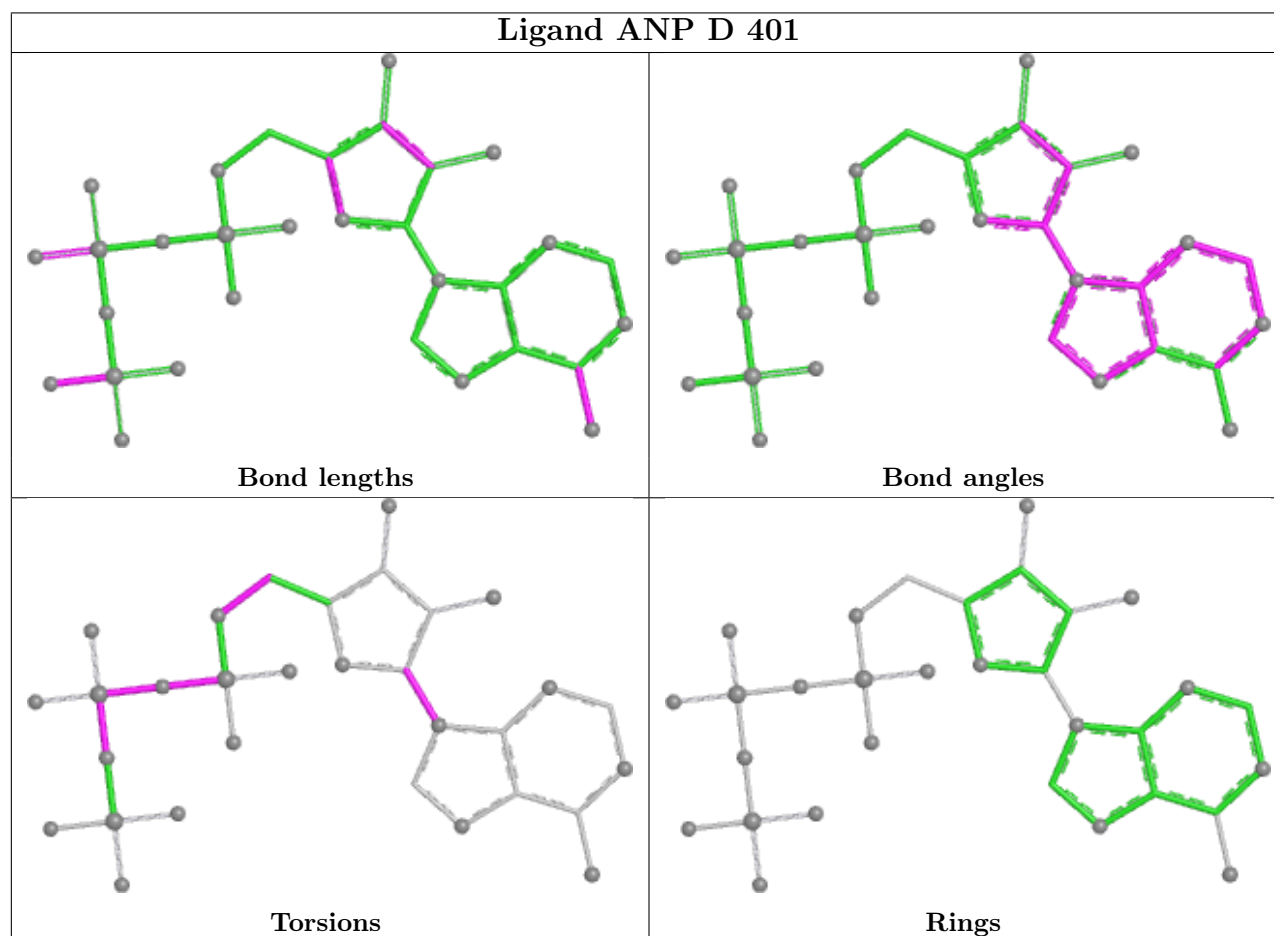
Mol	Chain	Res	Type	Atoms
2	A	1001	ANP	PG-N3B-PB-O1B
2	A	1001	ANP	PA-O3A-PB-O2B
2	B	401	ANP	PG-N3B-PB-O1B
2	B	401	ANP	PA-O3A-PB-O2B
2	B	401	ANP	C4'-C5'-O5'-PA
2	C	401	ANP	PG-N3B-PB-O1B
2	D	401	ANP	PG-N3B-PB-O1B
2	D	401	ANP	PA-O3A-PB-O2B
2	C	401	ANP	C2'-C1'-N9-C8
2	A	1001	ANP	PB-O3A-PA-O1A
2	D	401	ANP	PB-O3A-PA-O1A
2	D	401	ANP	C4'-C5'-O5'-PA
2	B	401	ANP	C2'-C1'-N9-C4
2	C	401	ANP	C2'-C1'-N9-C4
2	C	401	ANP	C4'-C5'-O5'-PA
2	D	401	ANP	C2'-C1'-N9-C8
2	B	401	ANP	C2'-C1'-N9-C8
2	D	401	ANP	C2'-C1'-N9-C4
2	A	1001	ANP	C4'-C5'-O5'-PA
2	A	1001	ANP	C2'-C1'-N9-C4
2	A	1001	ANP	C2'-C1'-N9-C8
2	C	401	ANP	PB-O3A-PA-O1A
2	A	1001	ANP	PA-O3A-PB-O1B
2	C	401	ANP	PA-O3A-PB-O1B
2	D	401	ANP	PA-O3A-PB-O1B
2	A	1001	ANP	O4'-C1'-N9-C8

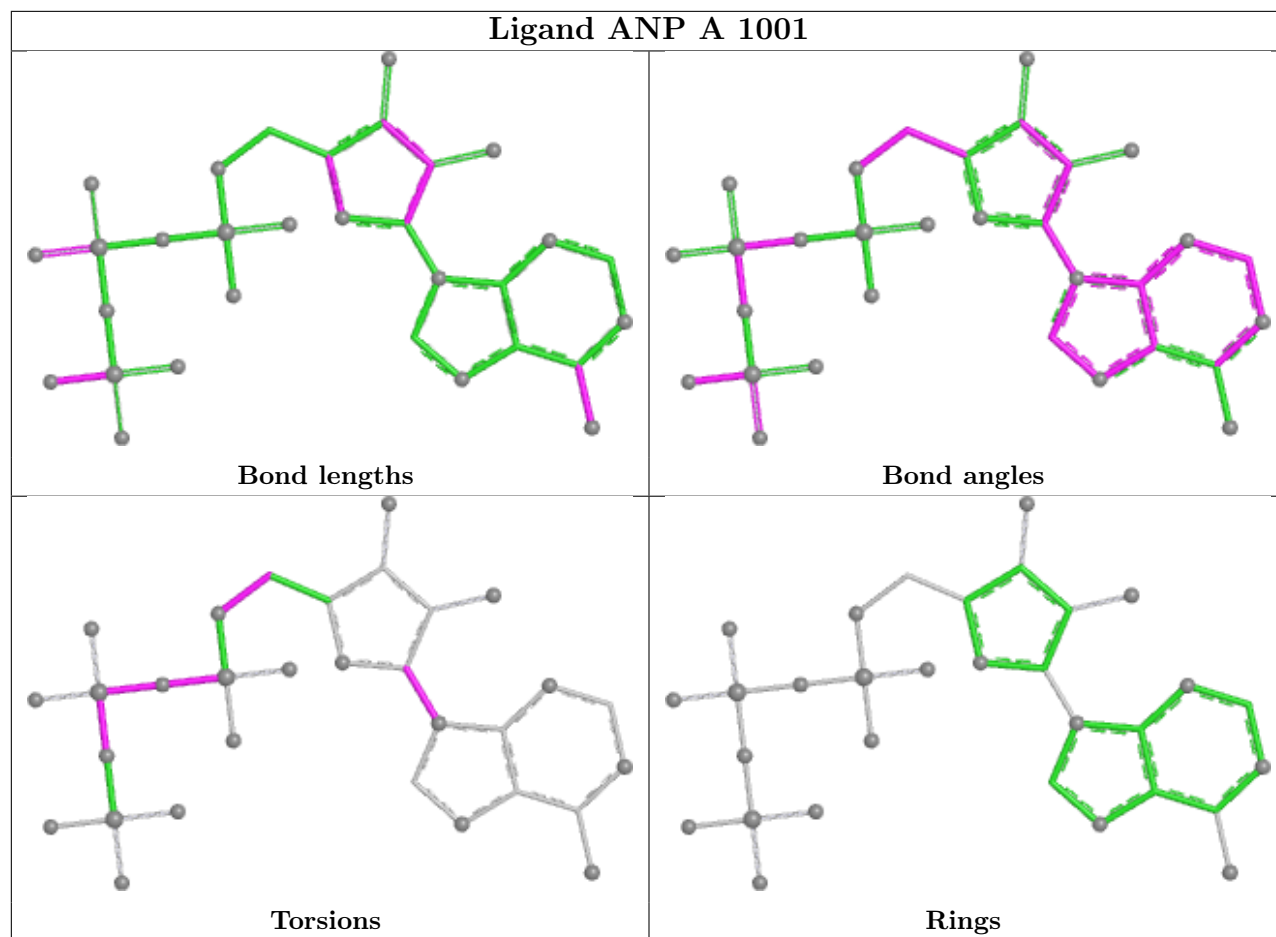
There are no ring outliers.

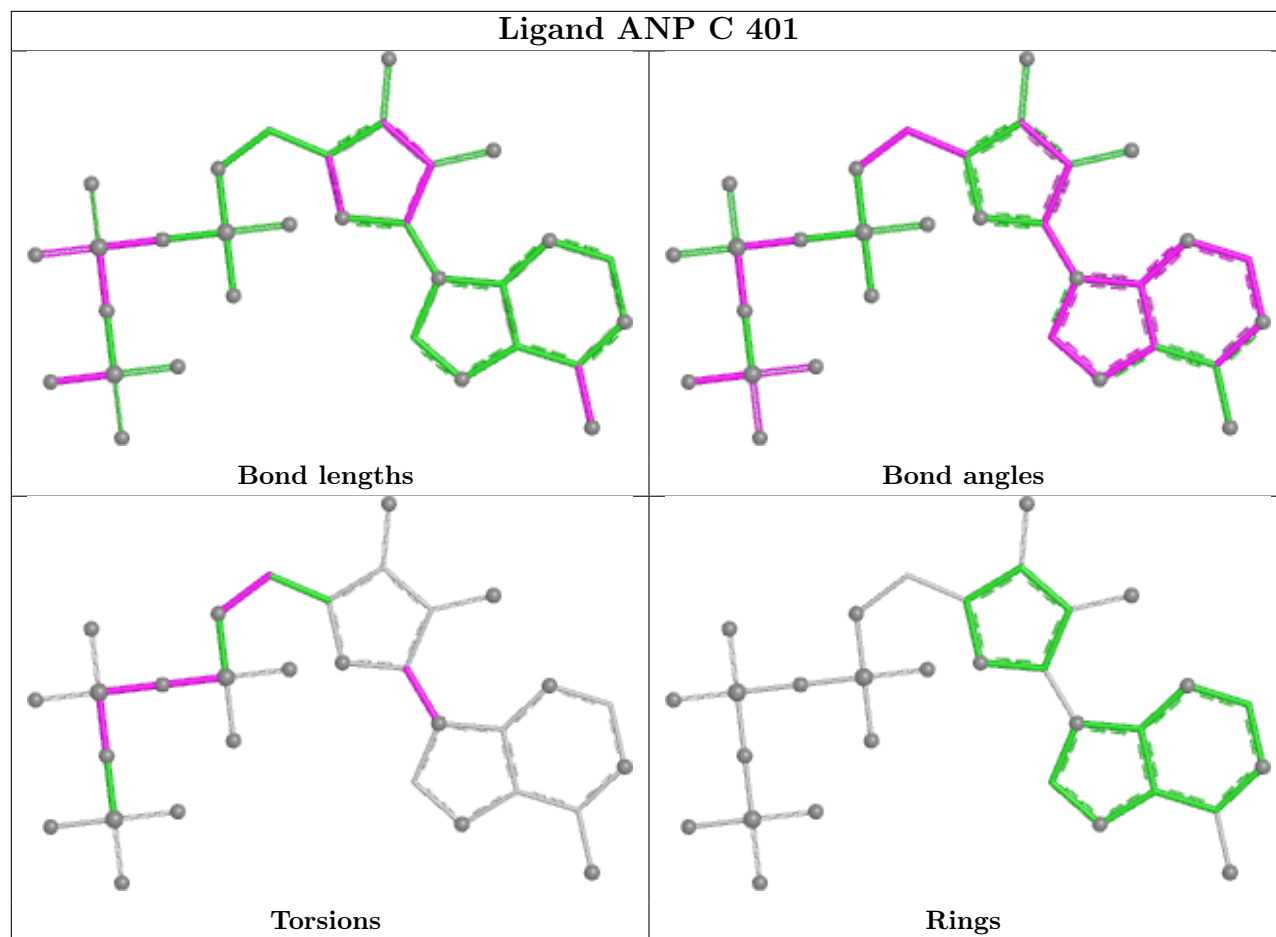
4 monomers are involved in 16 short contacts:

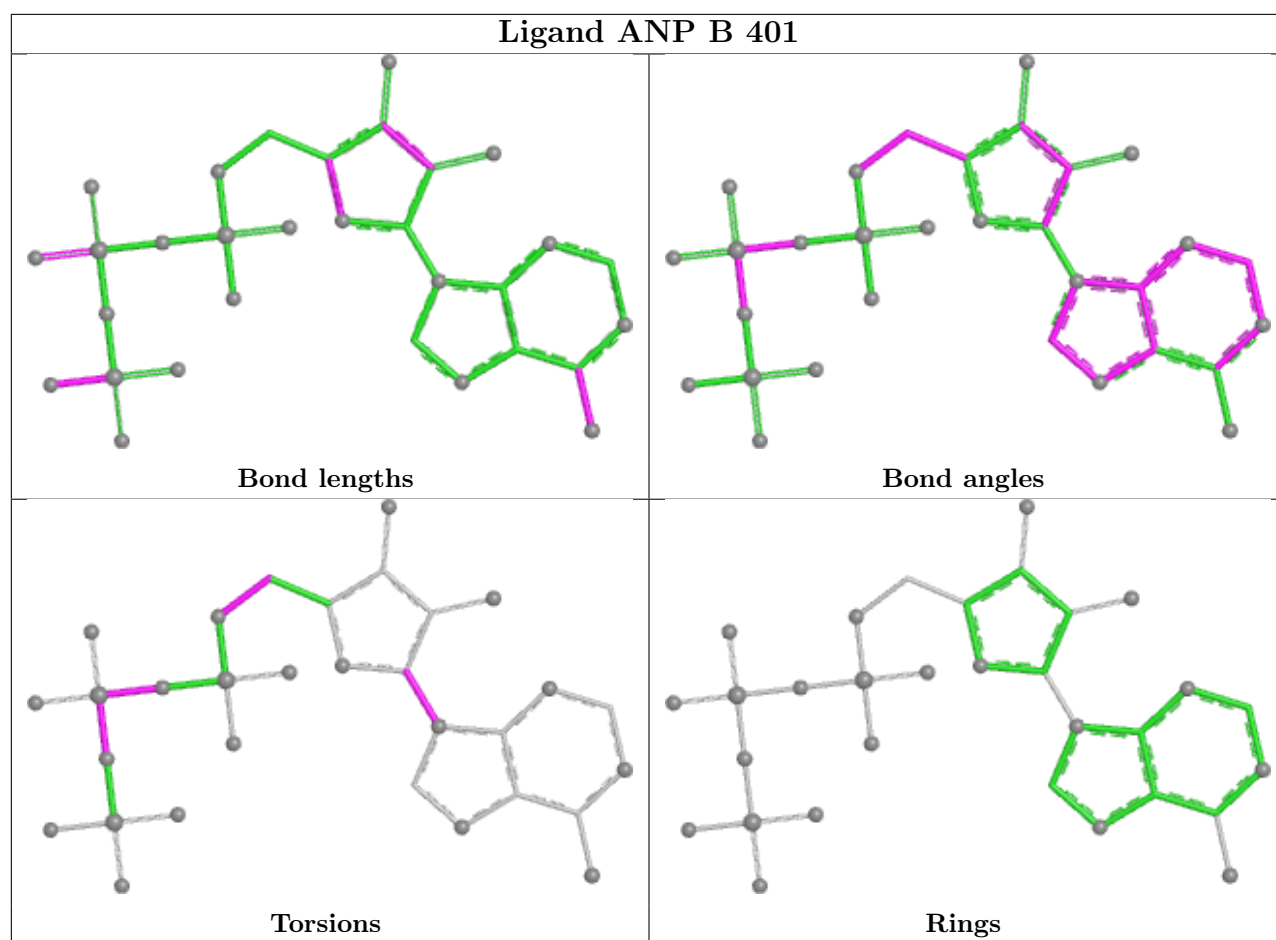
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	ANP	4	0
2	A	1001	ANP	1	0
2	C	401	ANP	5	0
2	B	401	ANP	6	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	285/317 (89%)	-0.15	3 (1%) 78 74	5, 16, 44, 68	0
1	B	285/317 (89%)	-0.11	6 (2%) 63 58	6, 18, 48, 68	0
1	C	316/317 (99%)	0.11	17 (5%) 31 26	6, 20, 70, 94	0
1	D	316/317 (99%)	0.09	22 (6%) 22 18	6, 20, 70, 90	0
All	All	1202/1268 (94%)	-0.01	48 (3%) 42 37	5, 18, 60, 94	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	ALA	5.8
1	B	165	VAL	5.5
1	A	165	VAL	5.1
1	C	145	LEU	4.2
1	C	158	ALA	4.0
1	D	150	PRO	4.0
1	D	142	ALA	4.0
1	B	132	PRO	3.9
1	D	134	GLY	3.6
1	D	140	GLN	3.3
1	C	142	ALA	3.3
1	D	135	ARG	3.1
1	D	151	GLY	3.1
1	C	137	TYR	3.0
1	C	150	PRO	3.0
1	D	145	LEU	3.0
1	D	137	TYR	3.0
1	B	167	PRO	3.0
1	C	136	PHE	3.0
1	D	158	ALA	2.9
1	C	144	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	133	VAL	2.8
1	A	316	ASP	2.7
1	C	146	MET	2.6
1	C	133	VAL	2.5
1	A	164	VAL	2.4
1	D	157	ASP	2.4
1	D	162	TRP	2.4
1	C	161	GLY	2.4
1	C	164	VAL	2.4
1	D	159	GLY	2.3
1	D	149	ASN	2.3
1	C	160	ARG	2.3
1	B	164	VAL	2.3
1	D	144	ASP	2.3
1	C	162	TRP	2.3
1	D	147	ALA	2.2
1	D	160	ARG	2.2
1	B	126	PHE	2.2
1	D	136	PHE	2.2
1	C	134	GLY	2.2
1	D	153	ILE	2.2
1	D	156	GLU	2.1
1	B	248	PRO	2.1
1	D	164	VAL	2.1
1	C	157	ASP	2.1
1	C	154	LEU	2.0
1	D	248	PRO	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.

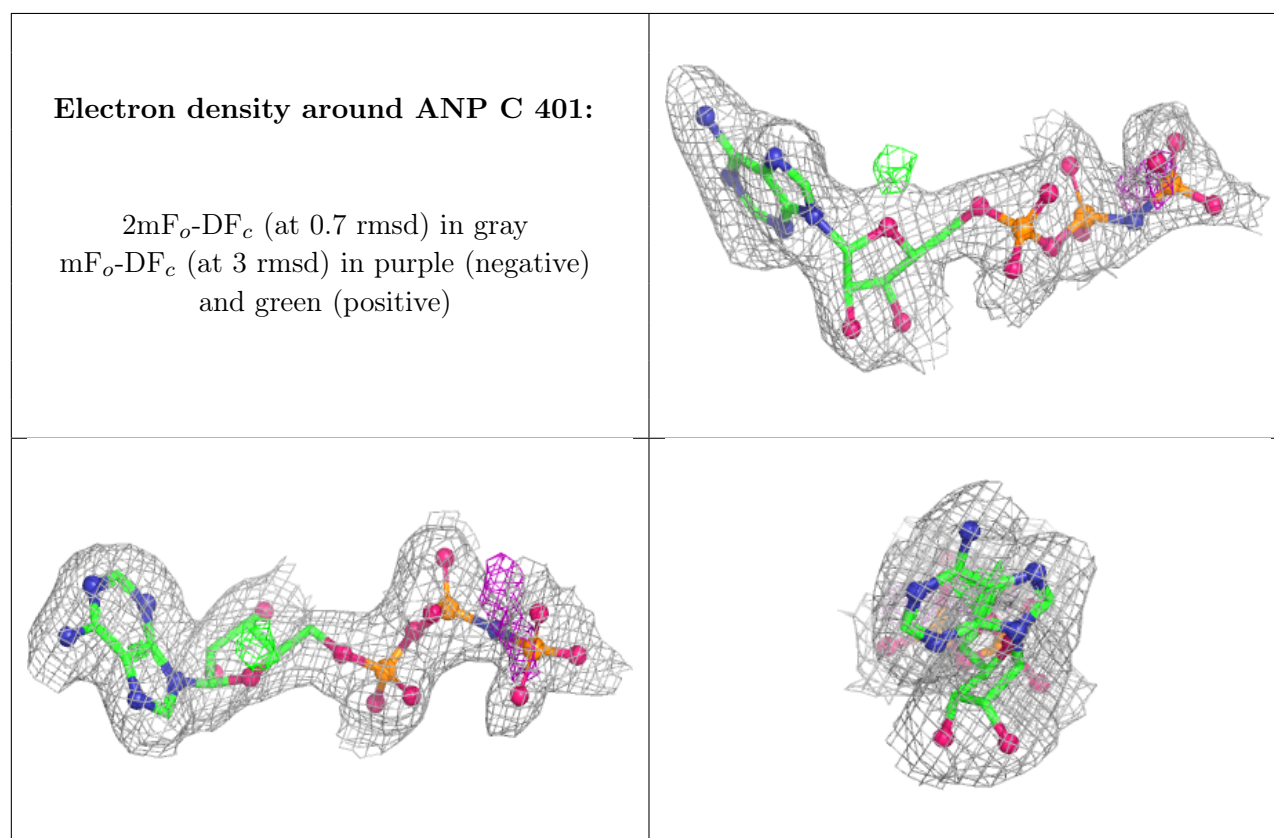
6.4 Ligands [i](#)

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.

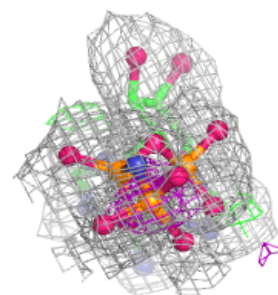
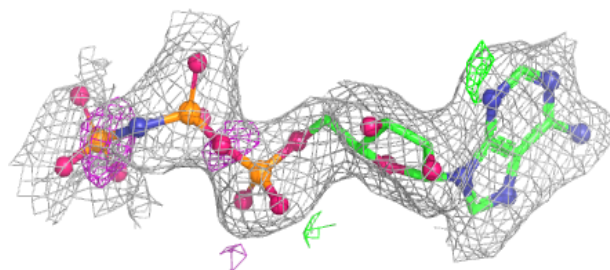
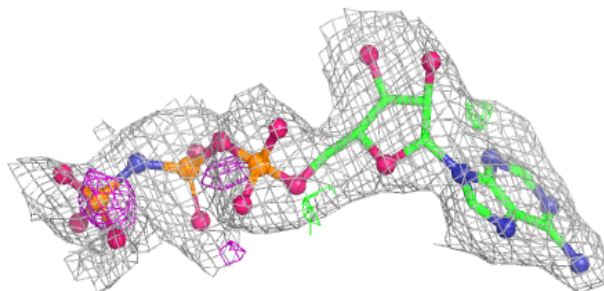
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ANP	C	401	31/31	0.89	0.10	15,29,42,77	0
2	ANP	B	401	31/31	0.91	0.11	15,28,38,82	0
2	ANP	A	1001	31/31	0.91	0.10	16,24,44,76	0
2	ANP	D	401	31/31	0.92	0.10	17,29,49,81	0

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.

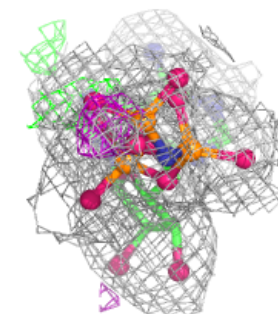
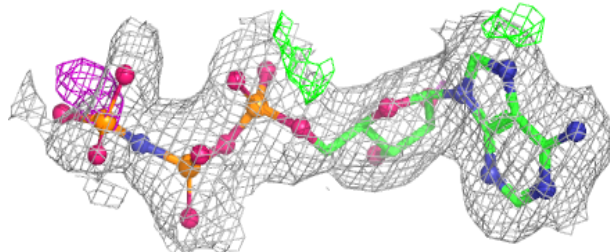
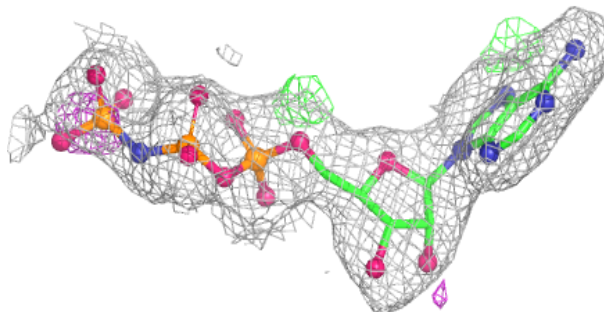


Electron density around ANP B 401:

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

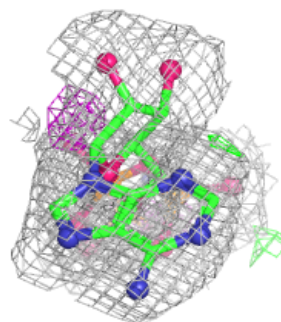
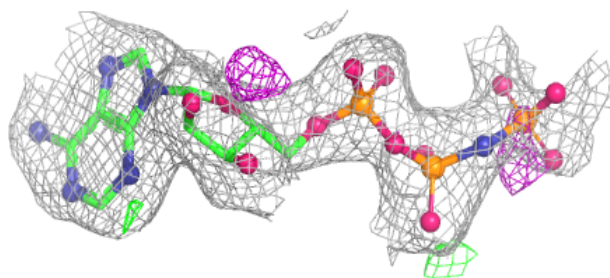
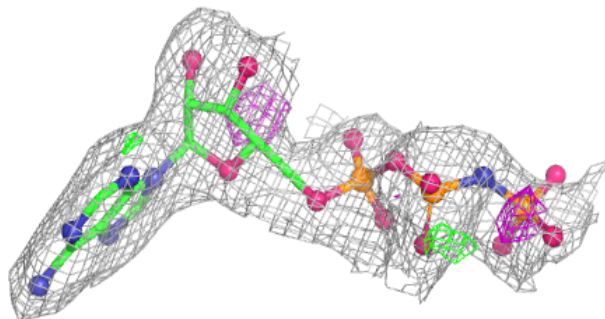
**Electron density around ANP A 1001:**

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



Electron density around ANP D 401:

$2mF_o - DF_c$ (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.