



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:09 AM UTC

PDB ID : 5C3Y / pdb_00005c3y
Title : Structure of human ribokinase crystallized with AMPPNP
Authors : Park, J.; Chakrabarti, J.; Singh, B.; Gupta, R.S.; Junop, M.S.
Deposited on : 2015-06-17
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

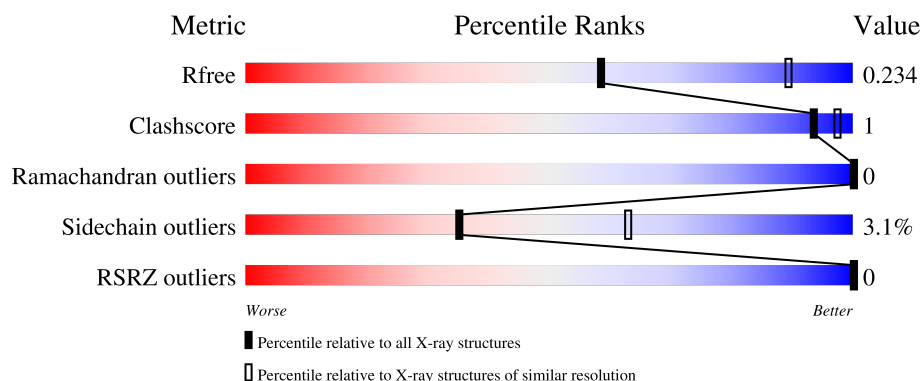
1 Overall quality at a glance

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	330	 88% . . 7%
1	B	330	 87% 6% . 5%
1	C	330	 87% 7% . 5%
1	D	330	 87% 6% . 6%
1	E	330	 85% 8% . 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	330	87% 6% • 5%
1	G	330	85% 8% • 5%
1	H	330	87% 7% 6%
1	I	330	88% 5% • 5%
1	J	330	89% 5% 5%
1	K	330	88% 5% 5%
1	L	330	88% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 28644 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 Ribokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	S	0	0	0
			2242	1414	371	443	14			
1	B	314	Total	C	N	O	S	0	1	0
			2313	1459	385	454	15			
1	C	313	Total	C	N	O	S	0	1	0
			2307	1454	383	455	15			
1	D	311	Total	C	N	O	S	0	1	0
			2281	1443	374	449	15			
1	E	311	Total	C	N	O	S	0	1	0
			2287	1447	372	453	15			
1	F	312	Total	C	N	O	S	0	0	0
			2292	1446	381	451	14			
1	G	314	Total	C	N	O	S	0	0	0
			2312	1460	383	455	14			
1	H	311	Total	C	N	O	S	0	0	0
			2275	1439	374	448	14			
1	I	313	Total	C	N	O	S	0	0	0
			2303	1453	384	452	14			
1	J	314	Total	C	N	O	S	0	0	0
			2289	1446	376	453	14			
1	K	312	Total	C	N	O	S	0	4	0
			2316	1463	380	457	16			
1	L	311	Total	C	N	O	S	0	1	0
			2269	1434	372	449	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	323	LEU	-	expression tag	UNP Q9H477
A	324	GLU	-	expression tag	UNP Q9H477
A	325	HIS	-	expression tag	UNP Q9H477
A	326	HIS	-	expression tag	UNP Q9H477
A	327	HIS	-	expression tag	UNP Q9H477

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	328	HIS	-	expression tag	UNP Q9H477
A	329	HIS	-	expression tag	UNP Q9H477
A	330	HIS	-	expression tag	UNP Q9H477
B	323	LEU	-	expression tag	UNP Q9H477
B	324	GLU	-	expression tag	UNP Q9H477
B	325	HIS	-	expression tag	UNP Q9H477
B	326	HIS	-	expression tag	UNP Q9H477
B	327	HIS	-	expression tag	UNP Q9H477
B	328	HIS	-	expression tag	UNP Q9H477
B	329	HIS	-	expression tag	UNP Q9H477
B	330	HIS	-	expression tag	UNP Q9H477
C	323	LEU	-	expression tag	UNP Q9H477
C	324	GLU	-	expression tag	UNP Q9H477
C	325	HIS	-	expression tag	UNP Q9H477
C	326	HIS	-	expression tag	UNP Q9H477
C	327	HIS	-	expression tag	UNP Q9H477
C	328	HIS	-	expression tag	UNP Q9H477
C	329	HIS	-	expression tag	UNP Q9H477
C	330	HIS	-	expression tag	UNP Q9H477
D	323	LEU	-	expression tag	UNP Q9H477
D	324	GLU	-	expression tag	UNP Q9H477
D	325	HIS	-	expression tag	UNP Q9H477
D	326	HIS	-	expression tag	UNP Q9H477
D	327	HIS	-	expression tag	UNP Q9H477
D	328	HIS	-	expression tag	UNP Q9H477
D	329	HIS	-	expression tag	UNP Q9H477
D	330	HIS	-	expression tag	UNP Q9H477
E	323	LEU	-	expression tag	UNP Q9H477
E	324	GLU	-	expression tag	UNP Q9H477
E	325	HIS	-	expression tag	UNP Q9H477
E	326	HIS	-	expression tag	UNP Q9H477
E	327	HIS	-	expression tag	UNP Q9H477
E	328	HIS	-	expression tag	UNP Q9H477
E	329	HIS	-	expression tag	UNP Q9H477
E	330	HIS	-	expression tag	UNP Q9H477
F	323	LEU	-	expression tag	UNP Q9H477
F	324	GLU	-	expression tag	UNP Q9H477
F	325	HIS	-	expression tag	UNP Q9H477
F	326	HIS	-	expression tag	UNP Q9H477
F	327	HIS	-	expression tag	UNP Q9H477
F	328	HIS	-	expression tag	UNP Q9H477
F	329	HIS	-	expression tag	UNP Q9H477

Continued on next page...

Continued from previous page...

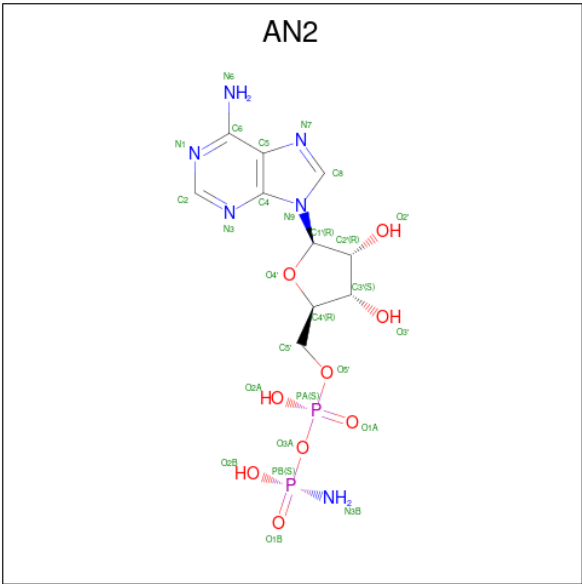
Chain	Residue	Modelled	Actual	Comment	Reference
F	330	HIS	-	expression tag	UNP Q9H477
G	323	LEU	-	expression tag	UNP Q9H477
G	324	GLU	-	expression tag	UNP Q9H477
G	325	HIS	-	expression tag	UNP Q9H477
G	326	HIS	-	expression tag	UNP Q9H477
G	327	HIS	-	expression tag	UNP Q9H477
G	328	HIS	-	expression tag	UNP Q9H477
G	329	HIS	-	expression tag	UNP Q9H477
G	330	HIS	-	expression tag	UNP Q9H477
H	323	LEU	-	expression tag	UNP Q9H477
H	324	GLU	-	expression tag	UNP Q9H477
H	325	HIS	-	expression tag	UNP Q9H477
H	326	HIS	-	expression tag	UNP Q9H477
H	327	HIS	-	expression tag	UNP Q9H477
H	328	HIS	-	expression tag	UNP Q9H477
H	329	HIS	-	expression tag	UNP Q9H477
H	330	HIS	-	expression tag	UNP Q9H477
I	323	LEU	-	expression tag	UNP Q9H477
I	324	GLU	-	expression tag	UNP Q9H477
I	325	HIS	-	expression tag	UNP Q9H477
I	326	HIS	-	expression tag	UNP Q9H477
I	327	HIS	-	expression tag	UNP Q9H477
I	328	HIS	-	expression tag	UNP Q9H477
I	329	HIS	-	expression tag	UNP Q9H477
I	330	HIS	-	expression tag	UNP Q9H477
J	323	LEU	-	expression tag	UNP Q9H477
J	324	GLU	-	expression tag	UNP Q9H477
J	325	HIS	-	expression tag	UNP Q9H477
J	326	HIS	-	expression tag	UNP Q9H477
J	327	HIS	-	expression tag	UNP Q9H477
J	328	HIS	-	expression tag	UNP Q9H477
J	329	HIS	-	expression tag	UNP Q9H477
J	330	HIS	-	expression tag	UNP Q9H477
K	323	LEU	-	expression tag	UNP Q9H477
K	324	GLU	-	expression tag	UNP Q9H477
K	325	HIS	-	expression tag	UNP Q9H477
K	326	HIS	-	expression tag	UNP Q9H477
K	327	HIS	-	expression tag	UNP Q9H477
K	328	HIS	-	expression tag	UNP Q9H477
K	329	HIS	-	expression tag	UNP Q9H477
K	330	HIS	-	expression tag	UNP Q9H477
L	323	LEU	-	expression tag	UNP Q9H477

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	324	GLU	-	expression tag	UNP Q9H477
L	325	HIS	-	expression tag	UNP Q9H477
L	326	HIS	-	expression tag	UNP Q9H477
L	327	HIS	-	expression tag	UNP Q9H477
L	328	HIS	-	expression tag	UNP Q9H477
L	329	HIS	-	expression tag	UNP Q9H477
L	330	HIS	-	expression tag	UNP Q9H477

- Molecule 2 is AMP PHOSPHORAMIDATE (CCD ID: AN2) (formula: C₁₀H₁₆N₆O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	E	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	F	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	G	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	H	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	I	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	J	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	K	1	Total	C	N	O	P	0	0
			27	10	6	9	2		
2	L	1	Total	C	N	O	P	0	0
			27	10	6	9	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		
3	B	2	Total	Na	0	0
			2	2		
3	C	2	Total	Na	0	0
			2	2		
3	D	2	Total	Na	0	0
			2	2		
3	E	2	Total	Na	0	0
			2	2		
3	F	2	Total	Na	0	0
			2	2		
3	G	2	Total	Na	0	0
			2	2		
3	H	2	Total	Na	0	0
			2	2		
3	I	2	Total	Na	0	0
			2	2		
3	J	2	Total	Na	0	0
			2	2		
3	K	2	Total	Na	0	0
			2	2		
3	L	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	56	Total	O	0	0
			56	56		

Continued on next page...

Continued from previous page...

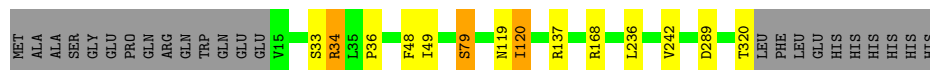
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	88	Total 88	O 88	0	0
4	C	96	Total 96	O 96	0	0
4	D	71	Total 71	O 71	0	0
4	E	90	Total 90	O 90	0	0
4	F	46	Total 46	O 46	0	0
4	G	83	Total 83	O 83	0	0
4	H	79	Total 79	O 79	0	0
4	I	54	Total 54	O 54	0	0
4	J	40	Total 40	O 40	0	0
4	K	58	Total 58	O 58	0	0
4	L	49	Total 49	O 49	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

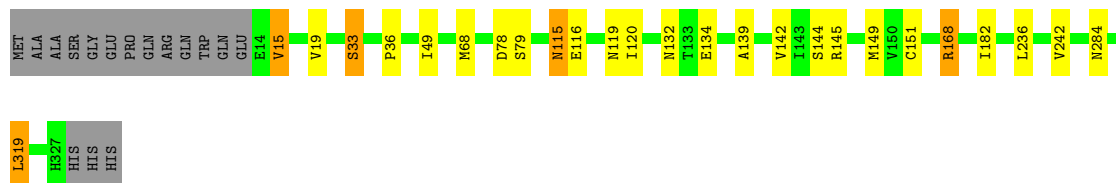
• Molecule 1: Ribokinase

Chain A:  88% 7%



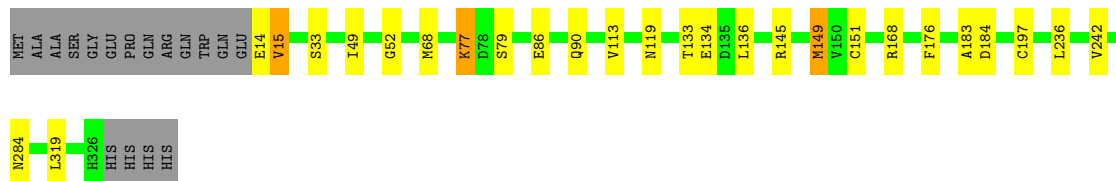
• Molecule 1: Ribokinase

Chain B:  87% 6% 5%



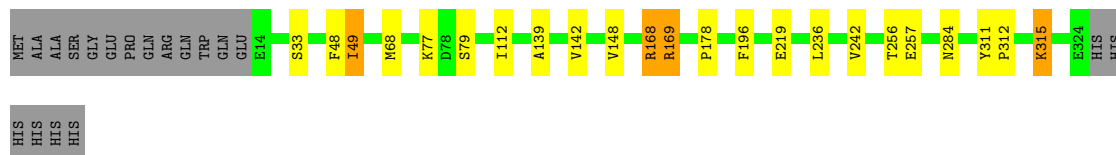
• Molecule 1: Ribokinase

Chain C:  87% 7% 5%



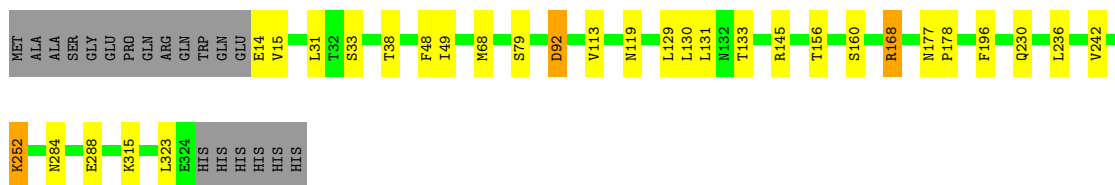
• Molecule 1: Ribokinase

Chain D:  87% 6% 6%



• Molecule 1: Ribokinase

Chain E:  85% 8% • 6%



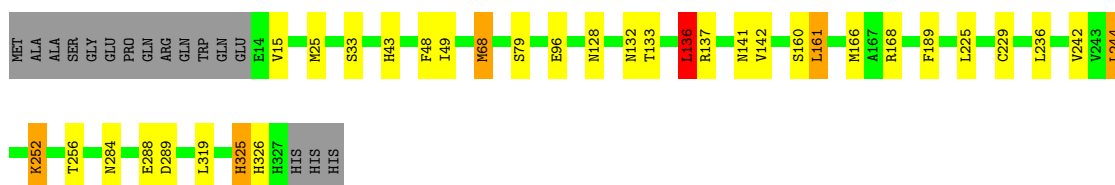
- Molecule 1: Ribokinase

Chain F:  87% 6% • 5%



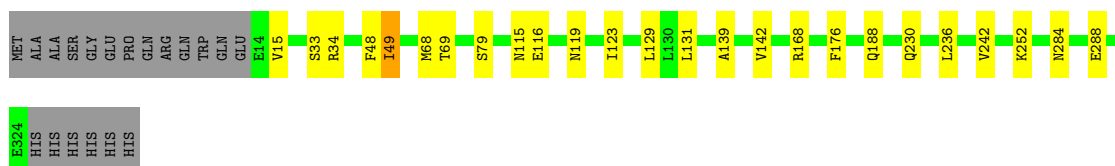
- Molecule 1: Ribokinase

Chain G:  85% 8% • 5%



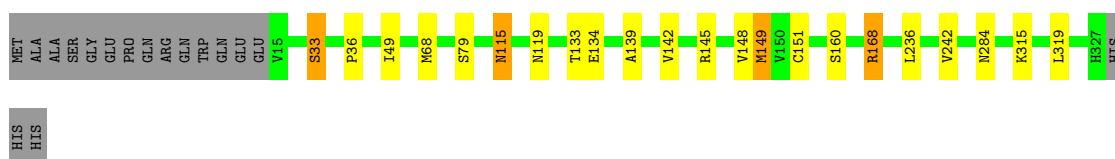
- Molecule 1: Ribokinase

Chain H:  87% 7% 6%



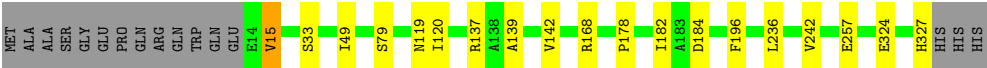
- Molecule 1: Ribokinase

Chain I:  88% 5% • 5%

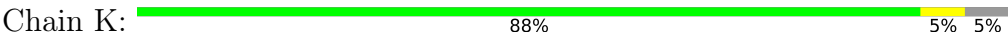


- Molecule 1: Ribokinase

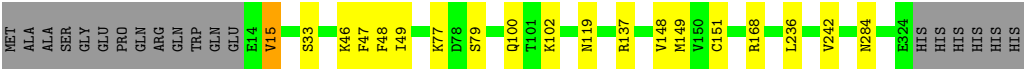
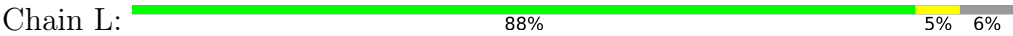
Chain J:  89% 5% 5%



● Molecule 1: Ribokinase



● Molecule 1: Ribokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.31Å 168.14Å 161.50Å 90.00° 90.82° 90.00°	Depositor
Resolution (Å)	51.26 – 2.60 51.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (51.26-2.60) 99.7 (51.26-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.205 , 0.232 0.209 , 0.234	Depositor DCC
R_{free} test set	6493 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 17.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,-l,-k 0.020 for -h,l,k 0.150 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28644	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AN2, NA

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	1.16	1/2274 (0.0%)	1.10	6/3095 (0.2%)
1	B	1.23	5/2348 (0.2%)	1.15	11/3197 (0.3%)
1	C	1.27	8/2341 (0.3%)	1.14	12/3187 (0.4%)
1	D	1.25	10/2314 (0.4%)	1.17	11/3150 (0.3%)
1	E	1.30	6/2320 (0.3%)	1.16	11/3158 (0.3%)
1	F	1.23	3/2326 (0.1%)	1.11	4/3167 (0.1%)
1	G	1.34	8/2347 (0.3%)	1.16	10/3194 (0.3%)
1	H	1.29	6/2308 (0.3%)	1.12	7/3143 (0.2%)
1	I	1.12	2/2339 (0.1%)	1.11	7/3185 (0.2%)
1	J	1.22	9/2323 (0.4%)	1.13	5/3166 (0.2%)
1	K	1.14	2/2351 (0.1%)	1.07	8/3202 (0.2%)
1	L	1.20	4/2302 (0.2%)	1.08	4/3138 (0.1%)
All	All	1.23	64/27893 (0.2%)	1.13	96/37982 (0.3%)

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	G	0	1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	115	ASN	CA-C	11.86	1.69	1.52
1	G	133	THR	CA-CB	9.64	1.68	1.53
1	J	15	VAL	CA-CB	9.46	1.65	1.54
1	C	183	ALA	CA-C	8.81	1.64	1.52
1	L	15	VAL	CA-CB	8.17	1.65	1.54
1	C	184	ASP	N-CA	7.76	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	92	ASP	CG-OD2	7.72	1.40	1.25
1	H	115	ASN	C-O	7.53	1.36	1.23
1	B	182	ILE	N-CA	7.41	1.55	1.46
1	J	257	GLU	CA-CB	7.14	1.65	1.53
1	E	133	THR	CA-CB	6.95	1.64	1.53
1	C	15	VAL	CA-CB	6.93	1.62	1.54
1	G	160	SER	C-O	-6.59	1.16	1.24
1	C	86	GLU	CD-OE2	6.59	1.37	1.25
1	F	96	GLU	CA-CB	6.49	1.63	1.53
1	B	182	ILE	CA-CB	6.39	1.62	1.54
1	D	257	GLU	CA-CB	6.35	1.63	1.53
1	J	327	HIS	CA-C	6.16	1.65	1.52
1	D	49	ILE	N-CA	-6.12	1.39	1.46
1	J	324	GLU	CA-C	6.08	1.61	1.52
1	D	49	ILE	CA-C	6.07	1.59	1.52
1	J	182	ILE	CA-CB	6.06	1.62	1.54
1	D	315	LYS	CA-CB	5.97	1.63	1.53
1	E	156	THR	CA-C	5.91	1.60	1.52
1	G	133	THR	N-CA	5.89	1.53	1.46
1	G	161	LEU	CA-CB	5.89	1.62	1.53
1	H	176	PHE	N-CA	5.79	1.53	1.46
1	D	256	THR	CA-C	5.61	1.59	1.52
1	D	77	LYS	CA-CB	5.49	1.59	1.52
1	L	77	LYS	CA-CB	5.45	1.59	1.52
1	K	257	GLU	N-CA	5.42	1.52	1.46
1	F	93	ILE	N-CA	-5.42	1.39	1.46
1	B	19	VAL	CA-C	-5.40	1.46	1.52
1	J	257	GLU	CA-C	5.37	1.59	1.52
1	C	90	GLN	CA-CB	5.33	1.61	1.53
1	G	132	ASN	CA-C	5.30	1.60	1.53
1	G	229	CYS	C-O	-5.29	1.17	1.23
1	C	14	GLU	CA-C	5.25	1.64	1.52
1	H	115	ASN	N-CA	5.23	1.53	1.46
1	D	169	ARG	CZ-NH2	5.22	1.40	1.33
1	B	78	ASP	CA-C	5.19	1.59	1.52
1	J	184	ASP	CA-CB	5.19	1.60	1.53
1	D	311	TYR	C-O	-5.18	1.17	1.24
1	J	182	ILE	N-CA	5.18	1.52	1.46
1	B	168	ARG	CZ-NH2	-5.17	1.26	1.33
1	E	131	LEU	C-O	-5.17	1.18	1.24
1	G	325	HIS	C-O	-5.15	1.17	1.23
1	L	137	ARG	N-CA	5.15	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	137	ARG	N-CA	5.15	1.52	1.46
1	H	49	ILE	C-O	-5.15	1.17	1.24
1	J	137	ARG	CA-CB	5.14	1.61	1.53
1	E	177	ASN	CA-C	5.13	1.57	1.52
1	L	100	GLN	C-O	-5.12	1.17	1.24
1	I	160	SER	C-O	-5.11	1.18	1.24
1	D	257	GLU	CA-C	5.10	1.59	1.52
1	E	160	SER	C-O	-5.08	1.18	1.24
1	A	137	ARG	CA-CB	5.06	1.61	1.53
1	H	131	LEU	C-O	-5.06	1.18	1.24
1	C	197	CYS	C-O	-5.05	1.18	1.24
1	F	77	LYS	CA-CB	5.04	1.59	1.52
1	D	112	ILE	C-O	-5.03	1.18	1.24
1	C	52	GLY	N-CA	5.01	1.49	1.44
1	K	163	ALA	CA-C	5.01	1.59	1.52
1	I	168	ARG	CZ-NH2	-5.00	1.26	1.33

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	ARG	NE-CZ-NH2	12.73	130.66	119.20
1	D	169	ARG	NE-CZ-NH1	-11.31	110.19	121.50
1	I	168	ARG	CD-NE-CZ	-11.27	108.63	124.40
1	B	168	ARG	CD-NE-CZ	-11.04	108.94	124.40
1	K	145	ARG	NE-CZ-NH1	-9.96	111.54	121.50
1	B	168	ARG	CA-CB-CG	-9.23	95.63	114.10
1	I	168	ARG	CA-CB-CG	-9.09	95.92	114.10
1	G	325	HIS	O-C-N	-9.06	112.52	122.85
1	A	34	ARG	CG-CD-NE	-8.37	93.59	112.00
1	I	315	LYS	CD-CE-NZ	7.79	136.83	111.90
1	L	15	VAL	CB-CA-C	-7.79	100.88	111.63
1	B	15	VAL	N-CA-C	7.64	120.49	108.87
1	C	184	ASP	CA-C-O	7.62	130.43	120.98
1	C	86	GLU	CB-CG-CD	7.42	125.22	112.60
1	J	324	GLU	N-CA-C	-7.18	103.18	112.23
1	H	15	VAL	N-CA-C	7.13	118.91	109.21
1	D	315	LYS	CA-CB-CG	7.13	128.37	114.10
1	H	115	ASN	CB-CA-C	-6.98	102.40	111.40
1	D	219	GLU	CG-CD-OE2	-6.96	102.40	118.40
1	C	15	VAL	CB-CA-C	-6.74	101.02	111.26
1	A	320	THR	N-CA-CB	-6.66	100.18	111.50
1	G	133	THR	N-CA-CB	6.63	119.87	110.12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	219	GLU	CG-CD-OE1	6.55	133.46	118.40
1	G	142	VAL	CB-CA-C	6.46	120.16	111.88
1	C	86	GLU	CA-CB-CG	-6.43	101.25	114.10
1	K	145	ARG	NE-CZ-NH2	6.31	124.88	119.20
1	J	257	GLU	CB-CA-C	6.27	119.68	109.90
1	E	48	PHE	N-CA-C	6.21	118.74	108.99
1	H	284	ASN	N-CA-C	6.16	120.53	112.89
1	K	119	ASN	N-CA-C	6.15	118.30	109.14
1	G	284	ASN	N-CA-C	6.12	120.58	113.18
1	L	48	PHE	N-CA-C	6.11	118.59	108.99
1	B	116	GLU	CB-CG-CD	6.10	122.97	112.60
1	B	116	GLU	CA-CB-CG	5.97	126.05	114.10
1	C	145	ARG	CG-CD-NE	-5.97	98.86	112.00
1	B	119	ASN	N-CA-C	5.96	118.03	109.14
1	I	168	ARG	NE-CZ-NH1	-5.95	115.55	121.50
1	I	134	GLU	CB-CG-CD	5.91	122.64	112.60
1	C	90	GLN	CB-CA-C	-5.84	101.09	110.79
1	E	15	VAL	N-CA-C	5.83	117.59	109.55
1	A	289	ASP	CB-CG-OD1	5.83	131.80	118.40
1	E	133	THR	N-CA-CB	5.81	118.67	110.12
1	A	120	ILE	CA-CB-CG1	5.80	120.27	110.40
1	J	15	VAL	CB-CA-C	-5.80	102.44	111.26
1	K	319	LEU	CA-CB-CG	5.80	136.59	116.30
1	C	119	ASN	N-CA-C	5.78	117.75	109.14
1	H	115	ASN	CA-C-O	5.78	131.54	121.38
1	G	142	VAL	CA-CB-CG1	5.77	120.20	110.40
1	F	141	ASN	CA-CB-CG	5.75	118.35	112.60
1	B	284	ASN	N-CA-C	5.69	120.06	113.18
1	E	119	ASN	N-CA-C	5.64	117.54	109.14
1	B	168	ARG	NE-CZ-NH1	-5.62	115.88	121.50
1	D	257	GLU	CB-CA-C	5.60	118.64	109.90
1	E	284	ASN	N-CA-C	5.59	119.72	113.01
1	G	48	PHE	N-CA-C	5.58	117.74	108.99
1	G	136	LEU	CA-CB-CG	5.56	135.75	116.30
1	D	49	ILE	CB-CA-C	5.51	119.19	110.81
1	K	284	ASN	N-CA-C	5.51	119.27	112.54
1	G	244	LEU	CB-CA-C	5.50	122.17	110.07
1	D	168	ARG	CG-CD-NE	-5.47	99.96	112.00
1	D	284	ASN	N-CA-C	5.46	119.79	113.18
1	F	119	ASN	N-CA-C	5.45	117.26	109.14
1	J	257	GLU	N-CA-CB	5.45	118.02	109.69
1	B	134	GLU	CA-CB-CG	-5.44	103.22	114.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	ALA	N-CA-C	-5.43	102.25	110.28
1	A	48	PHE	N-CA-C	5.42	117.50	108.99
1	D	48	PHE	N-CA-C	5.41	117.30	109.07
1	B	168	ARG	N-CA-C	5.41	116.86	111.07
1	E	113	VAL	CB-CA-C	5.41	118.23	110.33
1	A	119	ASN	N-CA-C	5.41	117.19	109.14
1	E	323	LEU	CA-C-N	5.38	131.38	121.70
1	E	323	LEU	C-N-CA	5.38	131.38	121.70
1	H	48	PHE	N-CA-C	5.36	117.41	108.99
1	H	119	ASN	N-CA-C	5.36	117.12	109.14
1	L	284	ASN	N-CA-C	5.34	119.64	113.18
1	B	319	LEU	N-CA-C	5.32	117.82	111.71
1	I	168	ARG	N-CA-C	5.30	116.75	111.07
1	E	14	GLU	CA-C-O	5.29	129.80	120.80
1	C	77	LYS	CB-CA-C	-5.28	103.50	112.00
1	K	168	ARG	CB-CA-C	-5.26	102.62	110.88
1	F	285	LEU	CA-CB-CG	5.23	134.62	116.30
1	K	145	ARG	CA-CB-CG	-5.21	103.69	114.10
1	C	284	ASN	N-CA-C	5.20	119.48	113.18
1	E	145	ARG	NE-CZ-NH1	-5.20	116.30	121.50
1	F	145	ARG	CG-CD-NE	5.19	123.41	112.00
1	I	119	ASN	N-CA-C	5.18	116.86	109.14
1	G	141	ASN	N-CA-C	5.18	116.74	111.14
1	J	119	ASN	N-CA-C	5.13	116.79	109.14
1	H	34	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	K	136	LEU	CA-CB-CG	5.08	134.08	116.30
1	C	136	LEU	CB-CA-C	-5.06	102.39	110.79
1	G	15	VAL	N-CA-C	5.06	116.10	109.21
1	D	168	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	E	168	ARG	CB-CA-C	-5.04	102.97	110.88
1	C	134	GLU	N-CA-C	5.03	116.76	111.28
1	L	119	ASN	N-CA-C	5.01	116.60	109.14

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	325	HIS	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	2242	0	2245	6	0
1	B	2313	0	2295	12	0
1	C	2307	0	2295	6	0
1	D	2281	0	2274	4	0
1	E	2287	0	2275	9	0
1	F	2292	0	2285	8	0
1	G	2312	0	2304	11	0
1	H	2275	0	2266	9	0
1	I	2303	0	2293	10	0
1	J	2289	0	2262	4	0
1	K	2316	0	2292	7	0
1	L	2269	0	2246	4	0
2	A	27	0	14	0	0
2	B	27	0	14	0	0
2	C	27	0	14	0	0
2	D	27	0	14	1	0
2	E	27	0	14	0	0
2	F	27	0	14	0	0
2	G	27	0	14	0	0
2	H	27	0	14	0	0
2	I	27	0	14	0	0
2	J	27	0	14	0	0
2	K	27	0	14	0	0
2	L	27	0	14	1	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	56	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	88	0	0	1	0
4	C	96	0	0	1	0
4	D	71	0	0	2	0
4	E	90	0	0	0	0
4	F	46	0	0	0	0
4	G	83	0	0	1	0
4	H	79	0	0	1	0
4	I	54	0	0	0	0
4	J	40	0	0	0	0
4	K	58	0	0	0	0
4	L	49	0	0	2	0
All	All	28644	0	27500	78	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 1.

All (78) 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:K:149:MET:HE1	1:K:151[A]:CYS:SG	2.21	0.81
1:B:145:ARG:NH1	1:E:129:LEU:HD13	1.96	0.80
1:B:149:MET:HE1	1:B:151:CYS:SG	2.22	0.79
1:I:149:MET:HE1	1:I:151:CYS:SG	2.22	0.79
1:C:149:MET:HE1	1:C:151[A]:CYS:SG	2.23	0.79
1:L:149:MET:HE1	1:L:151:CYS:SG	2.23	0.78
2:L:401:AN2:O1B	4:L:501:HOH:O	2.07	0.71
1:C:151[B]:CYS:SG	1:C:176:PHE:HD1	2.13	0.71
1:H:188:GLN:NE2	1:I:284:ASN:HD21	1.88	0.69
1:B:115:ASN:N	1:B:115:ASN:OD1	2.22	0.69
1:G:161:LEU:HG	1:G:189:PHE:CZ	2.29	0.67
1:F:141:ASN:OD1	1:F:145:ARG:NH2	2.28	0.66
1:E:315:LYS:HD3	1:G:96:GLU:CD	2.23	0.64
1:I:115:ASN:N	1:I:115:ASN:OD1	2.29	0.61
1:B:132:ASN:HB2	4:B:580:HOH:O	2.03	0.58
1:K:151[B]:CYS:SG	1:K:164:LEU:HD21	2.42	0.58
1:F:236:LEU:HD11	1:F:242:VAL:HG23	1.86	0.57
1:C:151[B]:CYS:HG	1:C:176:PHE:HD1	1.44	0.57
1:E:236:LEU:HD11	1:E:242:VAL:HG23	1.85	0.56
1:I:236:LEU:HD11	1:I:242:VAL:HG23	1.88	0.56
1:A:236:LEU:HD11	1:A:242:VAL:HG23	1.88	0.56
1:D:236:LEU:HD11	1:D:242:VAL:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:LYS:CB	4:L:542:HOH:O	2.55	0.55
1:B:236:LEU:HD11	1:B:242:VAL:HG23	1.89	0.55
1:H:236:LEU:HD11	1:H:242:VAL:HG23	1.88	0.55
1:F:34:ARG:HG3	1:F:34:ARG:HH21	1.71	0.54
1:C:236:LEU:HD11	1:C:242:VAL:HG23	1.88	0.54
1:E:68:MET:HA	1:E:68:MET:HE2	1.89	0.54
1:G:136:LEU:HD23	1:G:166:MET:SD	2.48	0.54
1:G:256:THR:HG21	4:G:507:HOH:O	2.08	0.54
1:J:236:LEU:HD11	1:J:242:VAL:HG23	1.91	0.53
1:K:236:LEU:HD11	1:K:242:VAL:HG23	1.89	0.53
1:L:236:LEU:HD11	1:L:242:VAL:HG23	1.90	0.53
1:G:236:LEU:HD11	1:G:242:VAL:HG23	1.89	0.53
1:C:151[B]:CYS:SG	1:C:176:PHE:CD1	2.97	0.52
1:G:252:LYS:HE3	1:G:288:GLU:OE1	2.09	0.52
1:E:252:LYS:HE3	1:E:288:GLU:OE1	2.10	0.52
1:G:225:LEU:HD22	1:G:244:LEU:HD13	1.91	0.52
1:H:188:GLN:HE21	1:I:284:ASN:HD21	1.54	0.52
1:E:38:THR:HG23	1:F:35:LEU:HD12	1.93	0.51
1:K:136:LEU:HD23	1:K:166[A]:MET:SD	2.50	0.51
1:B:15:VAL:HG21	1:B:145:ARG:CZ	2.41	0.50
1:A:120:ILE:HD12	1:B:36:PRO:HG2	1.95	0.49
2:D:401:AN2:O2B	4:D:501:HOH:O	2.20	0.49
1:G:43:HIS:HA	1:H:123:ILE:O	2.13	0.48
1:A:36:PRO:CG	1:B:120:ILE:HG23	2.44	0.48
1:K:136:LEU:HD23	1:K:166[B]:MET:SD	2.53	0.48
1:K:149:MET:HE3	1:K:149:MET:HB3	1.72	0.47
1:A:34:ARG:HD3	4:A:546:HOH:O	2.13	0.47
1:E:315:LYS:HB2	1:G:96:GLU:HG3	1.97	0.46
1:D:312:PRO:HA	4:D:507:HOH:O	2.16	0.46
1:H:252:LYS:HE2	1:H:288:GLU:OE1	2.16	0.45
1:I:33:SER:O	1:I:115:ASN:OD1	2.35	0.45
1:G:68:MET:HE3	1:G:68:MET:HA	1.98	0.45
1:K:139:ALA:O	1:K:142:VAL:HG12	2.17	0.45
1:B:33:SER:O	1:B:115:ASN:OD1	2.35	0.44
1:B:139:ALA:O	1:B:142:VAL:HG12	2.16	0.44
1:H:69:THR:N	4:H:502:HOH:O	2.38	0.44
1:J:139:ALA:O	1:J:142:VAL:HG12	2.17	0.44
1:A:36:PRO:HG2	1:B:120:ILE:HG23	1.99	0.44
1:C:68:MET:HG3	4:C:528:HOH:O	2.16	0.44
1:E:178:PRO:HG3	1:E:196:PHE:CZ	2.53	0.44
1:H:139:ALA:O	1:H:142:VAL:HG12	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:ALA:O	1:F:142:VAL:HG12	2.18	0.43
1:I:139:ALA:O	1:I:142:VAL:HG12	2.18	0.43
1:A:79:SER:HB3	4:A:539:HOH:O	2.18	0.43
1:F:178:PRO:HG3	1:F:196:PHE:CZ	2.53	0.43
1:H:188:GLN:NE2	1:I:284:ASN:ND2	2.62	0.42
1:D:139:ALA:O	1:D:142:VAL:HG12	2.19	0.42
1:D:178:PRO:HG3	1:D:196:PHE:CZ	2.54	0.42
1:G:25:MET:HE2	1:G:128:ASN:HD22	1.84	0.42
1:B:144:SER:OG	1:E:130:LEU:HD22	2.20	0.41
1:I:36:PRO:CG	1:J:120:ILE:HG23	2.51	0.41
1:H:129:LEU:HD13	1:I:145:ARG:NH1	2.35	0.41
1:F:34:ARG:HG3	1:F:34:ARG:NH2	2.33	0.41
1:L:46:LYS:HG3	1:L:47:PHE:N	2.35	0.41
1:J:178:PRO:HG3	1:J:196:PHE:CZ	2.56	0.40
1:F:285:LEU:HD11	1:F:289:ASP:OD2	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	304/330 (92%)	296 (97%)	8 (3%)	0	100	100
1	B	313/330 (95%)	305 (97%)	8 (3%)	0	100	100
1	C	312/330 (94%)	306 (98%)	6 (2%)	0	100	100
1	D	310/330 (94%)	303 (98%)	7 (2%)	0	100	100
1	E	310/330 (94%)	304 (98%)	6 (2%)	0	100	100
1	F	310/330 (94%)	302 (97%)	8 (3%)	0	100	100
1	G	312/330 (94%)	304 (97%)	8 (3%)	0	100	100
1	H	309/330 (94%)	301 (97%)	8 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	I	311/330 (94%)	303 (97%)	8 (3%)	0	100	100
1	J	312/330 (94%)	305 (98%)	7 (2%)	0	100	100
1	K	314/330 (95%)	307 (98%)	7 (2%)	0	100	100
1	L	310/330 (94%)	302 (97%)	8 (3%)	0	100	100
All	All	3727/3960 (94%)	3638 (98%)	89 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	240/266 (90%)	236 (98%)	4 (2%)	53	78
1	B	246/266 (92%)	239 (97%)	7 (3%)	38	66
1	C	247/266 (93%)	237 (96%)	10 (4%)	28	55
1	D	242/266 (91%)	234 (97%)	8 (3%)	33	61
1	E	243/266 (91%)	235 (97%)	8 (3%)	33	61
1	F	245/266 (92%)	236 (96%)	9 (4%)	30	57
1	G	247/266 (93%)	237 (96%)	10 (4%)	28	55
1	H	241/266 (91%)	234 (97%)	7 (3%)	37	65
1	I	247/266 (93%)	237 (96%)	10 (4%)	28	55
1	J	242/266 (91%)	237 (98%)	5 (2%)	47	73
1	K	247/266 (93%)	240 (97%)	7 (3%)	38	66
1	L	240/266 (90%)	234 (98%)	6 (2%)	42	69
All	All	2927/3192 (92%)	2836 (97%)	91 (3%)	35	63

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	49	ILE
1	A	79	SER
1	A	168	ARG
1	B	33	SER
1	B	49	ILE
1	B	68	MET
1	B	79	SER
1	B	115	ASN
1	B	168	ARG
1	B	319	LEU
1	C	15	VAL
1	C	33	SER
1	C	49	ILE
1	C	77	LYS
1	C	79	SER
1	C	113	VAL
1	C	133	THR
1	C	149	MET
1	C	168	ARG
1	C	319	LEU
1	D	33	SER
1	D	49	ILE
1	D	68	MET
1	D	79	SER
1	D	148	VAL
1	D	168	ARG
1	D	169	ARG
1	D	315	LYS
1	E	31	LEU
1	E	33	SER
1	E	49	ILE
1	E	79	SER
1	E	92	ASP
1	E	168	ARG
1	E	230	GLN
1	E	252	LYS
1	F	33	SER
1	F	49	ILE
1	F	77	LYS
1	F	79	SER
1	F	86	GLU
1	F	133	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	148	VAL
1	F	168	ARG
1	F	319	LEU
1	G	33	SER
1	G	49	ILE
1	G	68	MET
1	G	79	SER
1	G	136	LEU
1	G	168	ARG
1	G	252	LYS
1	G	289	ASP
1	G	319	LEU
1	G	326	HIS
1	H	33	SER
1	H	49	ILE
1	H	68	MET
1	H	79	SER
1	H	116	GLU
1	H	168	ARG
1	H	230	GLN
1	I	33	SER
1	I	49	ILE
1	I	68	MET
1	I	79	SER
1	I	115	ASN
1	I	133	THR
1	I	148	VAL
1	I	149	MET
1	I	168	ARG
1	I	319	LEU
1	J	15	VAL
1	J	33	SER
1	J	49	ILE
1	J	79	SER
1	J	168	ARG
1	K	33	SER
1	K	49	ILE
1	K	79	SER
1	K	136	LEU
1	K	148[A]	VAL
1	K	148[B]	VAL
1	K	168	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	15	VAL
1	L	33	SER
1	L	49	ILE
1	L	79	SER
1	L	148	VAL
1	L	168	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	43	HIS
1	C	230	GLN
1	C	284	ASN
1	D	45	HIS
1	D	87	ASN
1	D	308	GLN
1	E	87	ASN
1	E	141	ASN
1	E	308	GLN
1	F	43	HIS
1	G	43	HIS
1	H	87	ASN
1	H	188	GLN
1	H	230	GLN
1	H	308	GLN
1	I	45	HIS
1	K	90	GLN
1	L	45	HIS
1	L	253	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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
2	AN2	A	401	-	28,29,29	2.64	9 (32%)	40,45,45	2.10	13 (32%)
2	AN2	J	401	-	28,29,29	2.46	8 (28%)	40,45,45	2.04	14 (35%)
2	AN2	L	401	-	28,29,29	1.77	7 (25%)	40,45,45	2.05	14 (35%)
2	AN2	F	401	-	28,29,29	2.32	9 (32%)	40,45,45	1.96	14 (35%)
2	AN2	G	401	-	28,29,29	1.68	7 (25%)	40,45,45	2.00	7 (17%)
2	AN2	C	401	-	28,29,29	2.60	8 (28%)	40,45,45	2.07	12 (30%)
2	AN2	H	401	-	28,29,29	2.74	7 (25%)	40,45,45	2.08	10 (25%)
2	AN2	B	401	-	28,29,29	2.37	9 (32%)	40,45,45	1.77	7 (17%)
2	AN2	K	401	-	28,29,29	1.67	6 (21%)	40,45,45	2.02	11 (27%)
2	AN2	D	401	-	28,29,29	2.47	8 (28%)	40,45,45	1.93	9 (22%)
2	AN2	I	401	-	28,29,29	2.02	6 (21%)	40,45,45	1.90	10 (25%)
2	AN2	E	401	-	28,29,29	2.48	9 (32%)	40,45,45	1.93	10 (25%)

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	AN2	A	401	-	-	1/13/32/32	0/3/3/3
2	AN2	J	401	-	-	1/13/32/32	0/3/3/3
2	AN2	L	401	-	-	1/13/32/32	0/3/3/3
2	AN2	F	401	-	-	5/13/32/32	0/3/3/3
2	AN2	G	401	-	-	4/13/32/32	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AN2	C	401	-	-	1/13/32/32	0/3/3/3
2	AN2	H	401	-	-	0/13/32/32	0/3/3/3
2	AN2	B	401	-	-	1/13/32/32	0/3/3/3
2	AN2	K	401	-	-	3/13/32/32	0/3/3/3
2	AN2	D	401	-	-	0/13/32/32	0/3/3/3
2	AN2	I	401	-	-	2/13/32/32	0/3/3/3
2	AN2	E	401	-	-	0/13/32/32	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	401	AN2	PB-O1B	11.11	1.63	1.46
2	C	401	AN2	PB-O1B	10.53	1.62	1.46
2	A	401	AN2	PB-O1B	9.71	1.60	1.46
2	D	401	AN2	PB-O1B	8.92	1.59	1.46
2	E	401	AN2	PB-O1B	8.65	1.59	1.46
2	J	401	AN2	PA-O3A	7.77	1.67	1.59
2	F	401	AN2	PA-O3A	6.68	1.66	1.59
2	J	401	AN2	PB-O3A	6.16	1.66	1.59
2	B	401	AN2	PB-O3A	6.12	1.66	1.59
2	I	401	AN2	PA-O3A	5.58	1.65	1.59
2	F	401	AN2	PB-O3A	5.43	1.65	1.59
2	B	401	AN2	PA-O3A	5.42	1.65	1.59
2	F	401	AN2	C5-C4	5.05	1.48	1.39
2	B	401	AN2	C5-C4	5.04	1.48	1.39
2	E	401	AN2	C5-C4	4.98	1.48	1.39
2	I	401	AN2	C5-C4	4.98	1.48	1.39
2	D	401	AN2	C5-C4	4.96	1.47	1.39
2	L	401	AN2	C5-C4	4.94	1.47	1.39
2	H	401	AN2	PB-O3A	4.69	1.64	1.59
2	C	401	AN2	C5-C4	4.69	1.47	1.39
2	K	401	AN2	C5-C4	4.68	1.47	1.39
2	A	401	AN2	C5-C4	4.55	1.47	1.39
2	I	401	AN2	PB-O3A	4.49	1.64	1.59
2	A	401	AN2	PB-O3A	4.49	1.64	1.59
2	G	401	AN2	C5-C4	4.39	1.46	1.39
2	H	401	AN2	C5-N7	-4.33	1.31	1.39
2	J	401	AN2	C5-C4	4.25	1.46	1.39
2	A	401	AN2	PA-O3A	4.16	1.64	1.59
2	H	401	AN2	C5-C4	4.04	1.46	1.39
2	D	401	AN2	PB-O3A	4.02	1.64	1.59
2	J	401	AN2	PB-O1B	4.01	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	AN2	PB-O3A	3.87	1.63	1.59
2	E	401	AN2	PB-O3A	3.67	1.63	1.59
2	B	401	AN2	PB-O1B	3.63	1.51	1.46
2	G	401	AN2	PB-O1B	3.49	1.51	1.46
2	C	401	AN2	PB-O3A	3.32	1.63	1.59
2	E	401	AN2	C5-N7	-3.32	1.33	1.39
2	E	401	AN2	PA-O3A	3.31	1.63	1.59
2	D	401	AN2	PA-O3A	3.29	1.63	1.59
2	C	401	AN2	PA-O3A	3.26	1.63	1.59
2	K	401	AN2	PB-O1B	3.24	1.51	1.46
2	J	401	AN2	C5-C6	3.19	1.49	1.41
2	F	401	AN2	C4-N9	-3.18	1.31	1.37
2	B	401	AN2	C5-N7	-3.11	1.33	1.39
2	B	401	AN2	PB-O2B	3.07	1.65	1.56
2	I	401	AN2	PB-O1B	2.99	1.50	1.46
2	K	401	AN2	PA-O3A	2.98	1.62	1.59
2	I	401	AN2	C5-N7	-2.90	1.33	1.39
2	G	401	AN2	PB-O3A	2.87	1.62	1.59
2	D	401	AN2	C5-C6	2.86	1.48	1.41
2	F	401	AN2	C5-N7	-2.85	1.33	1.39
2	C	401	AN2	C5-N7	-2.83	1.33	1.39
2	H	401	AN2	PB-O2B	-2.81	1.49	1.56
2	G	401	AN2	C5-N7	-2.80	1.34	1.39
2	J	401	AN2	C8-N7	2.79	1.37	1.31
2	B	401	AN2	C5-C6	2.78	1.48	1.41
2	E	401	AN2	C4-N9	-2.78	1.31	1.37
2	F	401	AN2	C5-C6	2.74	1.48	1.41
2	D	401	AN2	C4-N9	-2.73	1.32	1.37
2	L	401	AN2	C5-N7	-2.72	1.34	1.39
2	L	401	AN2	C5-C6	2.72	1.48	1.41
2	A	401	AN2	C5-C6	2.72	1.48	1.41
2	B	401	AN2	C4-N9	-2.68	1.32	1.37
2	E	401	AN2	PB-O2B	-2.63	1.49	1.56
2	G	401	AN2	C5-C6	2.61	1.48	1.41
2	E	401	AN2	C8-N7	2.57	1.36	1.31
2	A	401	AN2	C5-N7	-2.56	1.34	1.39
2	D	401	AN2	C5-N7	-2.50	1.34	1.39
2	F	401	AN2	PB-O1B	2.49	1.49	1.46
2	F	401	AN2	PB-O2B	2.44	1.63	1.56
2	B	401	AN2	C8-N7	2.42	1.36	1.31
2	A	401	AN2	PB-O2B	-2.40	1.50	1.56
2	J	401	AN2	C4-N9	-2.37	1.32	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	401	AN2	C5-C6	2.36	1.47	1.41
2	L	401	AN2	PB-O1B	2.31	1.49	1.46
2	C	401	AN2	C5-C6	2.31	1.47	1.41
2	A	401	AN2	C8-N7	2.31	1.36	1.31
2	H	401	AN2	C8-N7	2.30	1.36	1.31
2	K	401	AN2	PB-O3A	2.29	1.61	1.59
2	E	401	AN2	C5-C6	2.29	1.47	1.41
2	D	401	AN2	PB-O2B	-2.27	1.50	1.56
2	K	401	AN2	C5-N7	-2.24	1.35	1.39
2	H	401	AN2	C4-N9	-2.21	1.33	1.37
2	C	401	AN2	C8-N7	2.21	1.35	1.31
2	C	401	AN2	C4-N9	-2.19	1.33	1.37
2	L	401	AN2	C8-N7	2.12	1.35	1.31
2	G	401	AN2	C4-N9	-2.11	1.33	1.37
2	L	401	AN2	PB-O2B	2.11	1.62	1.56
2	F	401	AN2	C8-N7	2.10	1.35	1.31
2	I	401	AN2	C8-N7	2.07	1.35	1.31
2	G	401	AN2	C8-N7	2.06	1.35	1.31
2	J	401	AN2	PB-O2B	2.03	1.62	1.56
2	A	401	AN2	C4-N9	-2.01	1.33	1.37

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	AN2	C5-C4-N3	-6.39	117.91	126.72
2	H	401	AN2	C5-C4-N3	-6.27	118.08	126.72
2	D	401	AN2	C5-C4-N3	-6.01	118.44	126.72
2	E	401	AN2	C5-C4-N3	-5.82	118.71	126.72
2	K	401	AN2	C5-C4-N3	-5.64	118.95	126.72
2	A	401	AN2	C5-C4-N3	-5.63	118.97	126.72
2	K	401	AN2	N3-C4-N9	5.43	136.40	127.17
2	D	401	AN2	N3-C4-N9	5.34	136.24	127.17
2	I	401	AN2	C5-C4-N3	-5.25	119.48	126.72
2	L	401	AN2	C5-C4-N3	-5.20	119.56	126.72
2	H	401	AN2	N3-C4-N9	5.18	135.98	127.17
2	F	401	AN2	C5-C4-N3	-5.01	119.82	126.72
2	C	401	AN2	C5-C4-N3	-4.93	119.93	126.72
2	J	401	AN2	C5-C4-N3	-4.87	120.02	126.72
2	B	401	AN2	C5-C4-N3	-4.87	120.02	126.72
2	C	401	AN2	O2B-PB-O3A	4.84	120.81	104.64
2	C	401	AN2	N1-C2-N3	-4.67	121.52	128.58
2	I	401	AN2	N3-C4-N9	4.65	135.07	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	AN2	N3-C4-N9	4.57	134.93	127.17
2	C	401	AN2	N3-C4-N9	4.56	134.92	127.17
2	G	401	AN2	N3-C4-N9	4.53	134.88	127.17
2	J	401	AN2	N1-C2-N3	-4.52	121.74	128.58
2	E	401	AN2	N3-C4-N9	4.47	134.76	127.17
2	A	401	AN2	N3-C4-N9	4.41	134.67	127.17
2	H	401	AN2	N1-C2-N3	-4.35	121.99	128.58
2	J	401	AN2	C2-N3-C4	4.24	122.18	111.83
2	K	401	AN2	N1-C2-N3	-4.20	122.23	128.58
2	G	401	AN2	C2-N3-C4	4.19	122.05	111.83
2	L	401	AN2	N1-C2-N3	-4.18	122.25	128.58
2	H	401	AN2	C2-N3-C4	4.15	121.95	111.83
2	G	401	AN2	N1-C2-N3	-4.08	122.41	128.58
2	B	401	AN2	O2B-PB-O3A	4.03	118.09	104.64
2	C	401	AN2	C2-N3-C4	3.97	121.53	111.83
2	A	401	AN2	C2-N3-C4	3.96	121.49	111.83
2	K	401	AN2	C2-N3-C4	3.87	121.28	111.83
2	L	401	AN2	C2-N3-C4	3.86	121.26	111.83
2	A	401	AN2	N1-C2-N3	-3.85	122.75	128.58
2	E	401	AN2	O2B-PB-O3A	3.76	117.20	104.64
2	F	401	AN2	N3-C4-N9	3.74	133.53	127.17
2	I	401	AN2	N1-C2-N3	-3.74	122.93	128.58
2	E	401	AN2	C2-N3-C4	3.61	120.64	111.83
2	F	401	AN2	O2A-PA-O1A	3.59	129.14	112.44
2	G	401	AN2	C4-C5-N7	-3.56	106.51	110.58
2	J	401	AN2	C6-C5-N7	3.52	138.87	132.09
2	D	401	AN2	C2-N3-C4	3.49	120.35	111.83
2	A	401	AN2	O2B-PB-O3A	3.47	116.22	104.64
2	B	401	AN2	N1-C2-N3	-3.44	123.37	128.58
2	H	401	AN2	O2B-PB-O3A	3.43	116.10	104.64
2	F	401	AN2	N1-C2-N3	-3.38	123.47	128.58
2	A	401	AN2	C4-C5-N7	-3.37	106.73	110.58
2	F	401	AN2	C2-N3-C4	3.36	120.05	111.83
2	E	401	AN2	N1-C2-N3	-3.35	123.50	128.58
2	B	401	AN2	C2-N3-C4	3.33	119.97	111.83
2	I	401	AN2	O5'-PA-O1A	-3.33	95.72	108.94
2	J	401	AN2	C4-C5-N7	-3.28	106.84	110.58
2	K	401	AN2	C4-N9-C8	3.27	109.17	105.74
2	F	401	AN2	C4-C5-N7	-3.27	106.84	110.58
2	J	401	AN2	N3-C4-N9	3.26	132.71	127.17
2	I	401	AN2	C2-N3-C4	3.26	119.78	111.83
2	B	401	AN2	C4-C5-N7	-3.21	106.91	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	AN2	O3A-PA-O1A	-3.15	101.24	110.70
2	F	401	AN2	O2B-PB-O3A	3.11	115.03	104.64
2	H	401	AN2	O3A-PA-O1A	-3.08	101.42	110.70
2	B	401	AN2	N3-C4-N9	3.08	132.41	127.17
2	J	401	AN2	O2A-PA-O3A	3.07	115.56	107.27
2	C	401	AN2	C2'-C1'-N9	-3.03	105.77	113.30
2	L	401	AN2	PB-O3A-PA	-3.00	122.50	132.10
2	D	401	AN2	O2B-PB-O3A	2.94	114.45	104.64
2	D	401	AN2	O2A-PA-O3A	2.92	115.18	107.27
2	D	401	AN2	N1-C2-N3	-2.84	124.28	128.58
2	I	401	AN2	C2-N1-C6	2.83	123.39	118.73
2	L	401	AN2	O4'-C1'-N9	2.83	113.53	108.09
2	H	401	AN2	O2A-PA-O1A	2.79	125.41	112.44
2	L	401	AN2	C3'-C2'-C1'	2.75	106.67	101.46
2	D	401	AN2	N6-C6-N1	2.64	124.25	118.38
2	A	401	AN2	C4-N9-C8	2.62	108.49	105.74
2	A	401	AN2	O2A-PA-O1A	2.62	124.62	112.44
2	A	401	AN2	C5-N7-C8	2.61	107.56	103.45
2	G	401	AN2	PB-O3A-PA	-2.56	123.92	132.10
2	A	401	AN2	C6-C5-N7	2.56	137.02	132.09
2	H	401	AN2	PB-O3A-PA	-2.51	124.09	132.10
2	I	401	AN2	N6-C6-N1	2.49	123.93	118.38
2	H	401	AN2	C5-C6-N6	-2.46	117.19	123.29
2	C	401	AN2	C4-N9-C8	2.46	108.32	105.74
2	B	401	AN2	C6-C5-N7	2.45	136.82	132.09
2	E	401	AN2	C4-C5-N7	-2.45	107.79	110.58
2	G	401	AN2	C5-N7-C8	2.44	107.28	103.45
2	J	401	AN2	C4-N9-C8	2.41	108.27	105.74
2	E	401	AN2	O2A-PA-O1A	2.41	123.67	112.44
2	K	401	AN2	N6-C6-N1	2.39	123.70	118.38
2	F	401	AN2	C4-N9-C8	2.38	108.24	105.74
2	A	401	AN2	O2A-PA-O3A	2.38	113.72	107.27
2	J	401	AN2	C4-N9-C1'	-2.33	121.18	126.63
2	C	401	AN2	C5-C6-N6	-2.29	117.62	123.29
2	L	401	AN2	C2-N1-C6	2.28	122.48	118.73
2	L	401	AN2	C4-N9-C8	2.28	108.13	105.74
2	J	401	AN2	C2-N1-C6	2.27	122.46	118.73
2	F	401	AN2	O5'-C5'-C4'	2.27	116.71	108.99
2	K	401	AN2	C5-C6-N6	-2.26	117.69	123.29
2	K	401	AN2	O5'-PA-O1A	-2.25	100.00	108.94
2	L	401	AN2	C4-C5-N7	-2.25	108.01	110.58
2	A	401	AN2	O5'-C5'-C4'	2.25	116.64	108.99

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	AN2	N6-C6-N1	2.24	123.37	118.38
2	L	401	AN2	O2B-PB-O1B	2.24	116.06	110.26
2	L	401	AN2	O2'-C2'-C1'	-2.24	102.40	110.10
2	I	401	AN2	PB-O3A-PA	-2.23	124.96	132.10
2	E	401	AN2	O2B-PB-O1B	-2.22	104.53	110.26
2	F	401	AN2	C6-C5-N7	2.19	136.30	132.09
2	C	401	AN2	C2-N1-C6	2.18	122.31	118.73
2	F	401	AN2	C2-N1-C6	2.16	122.28	118.73
2	A	401	AN2	N9-C8-N7	-2.16	110.87	113.94
2	J	401	AN2	N9-C8-N7	-2.15	110.89	113.94
2	E	401	AN2	C3'-C2'-C1'	2.14	105.51	101.46
2	I	401	AN2	O2A-PA-O1A	2.14	122.39	112.44
2	C	401	AN2	PB-O3A-PA	-2.12	125.32	132.10
2	C	401	AN2	O4'-C1'-N9	2.12	112.16	108.09
2	J	401	AN2	C6-C5-C4	-2.11	114.29	117.18
2	K	401	AN2	C4-C5-N7	-2.11	108.17	110.58
2	D	401	AN2	C4-N9-C8	2.11	107.95	105.74
2	L	401	AN2	O5'-PA-O1A	-2.10	100.62	108.94
2	J	401	AN2	C5-N7-C8	2.09	106.74	103.45
2	F	401	AN2	C5-N7-C8	2.09	106.73	103.45
2	K	401	AN2	C2-N1-C6	2.08	122.15	118.73
2	K	401	AN2	C5-N7-C8	2.07	106.71	103.45
2	E	401	AN2	N6-C6-N1	2.07	122.99	118.38
2	J	401	AN2	O5'-PA-O1A	-2.07	100.75	108.94
2	D	401	AN2	C5-C6-N6	-2.06	118.19	123.29
2	F	401	AN2	O4'-C4'-C5'	2.05	115.90	109.33
2	L	401	AN2	N6-C6-N1	2.04	122.92	118.38
2	C	401	AN2	N6-C6-N1	2.03	122.91	118.38
2	I	401	AN2	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	401	AN2	C5'-O5'-PA-O3A
2	F	401	AN2	C5'-O5'-PA-O2A
2	G	401	AN2	C5'-O5'-PA-O3A
2	G	401	AN2	C5'-O5'-PA-O1A
2	G	401	AN2	C5'-O5'-PA-O2A
2	F	401	AN2	O4'-C4'-C5'-O5'
2	F	401	AN2	C3'-C4'-C5'-O5'
2	B	401	AN2	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	F	401	AN2	PB-O3A-PA-O1A
2	I	401	AN2	C5'-O5'-PA-O1A
2	K	401	AN2	C5'-O5'-PA-O1A
2	C	401	AN2	O4'-C4'-C5'-O5'
2	K	401	AN2	PB-O3A-PA-O2A
2	A	401	AN2	PB-O3A-PA-O2A
2	G	401	AN2	PB-O3A-PA-O2A
2	L	401	AN2	PB-O3A-PA-O2A
2	I	401	AN2	PB-O3A-PA-O1A
2	J	401	AN2	PB-O3A-PA-O1A
2	K	401	AN2	PB-O3A-PA-O1A

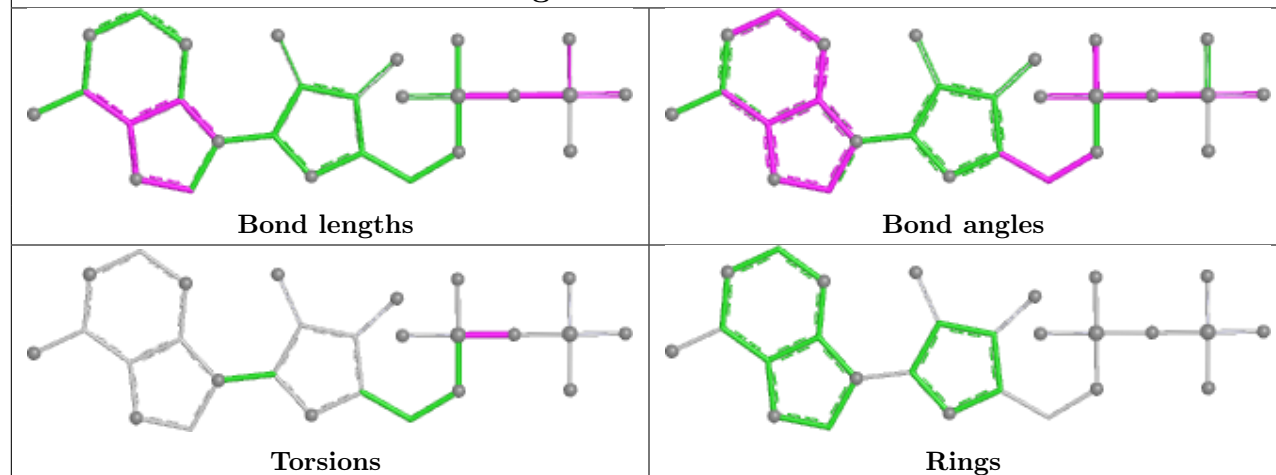
There are no ring outliers.

2 monomers are involved in 2 short contacts:

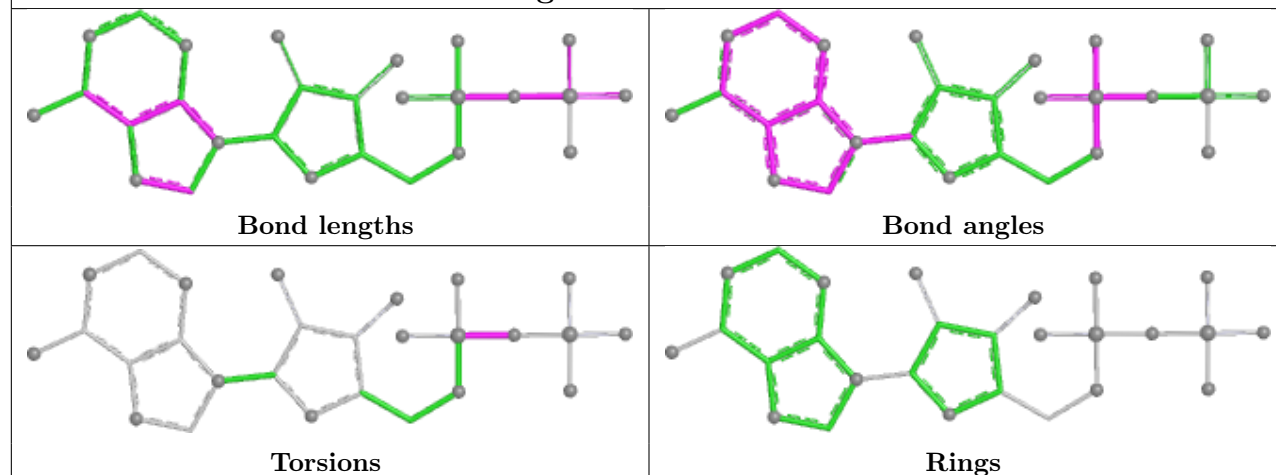
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	AN2	1	0
2	D	401	AN2	1	0

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.

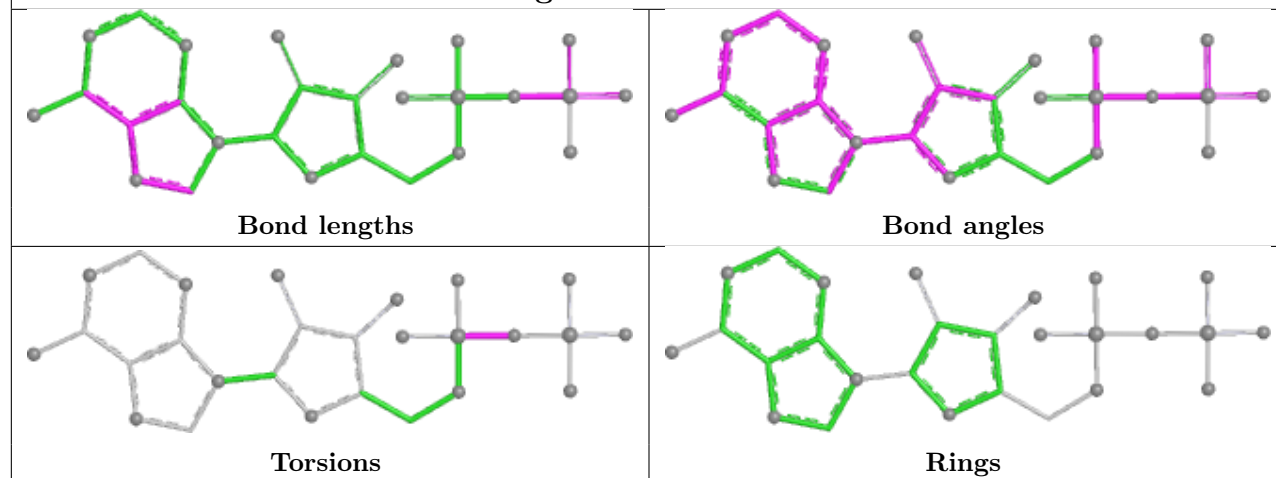
Ligand AN2 A 401



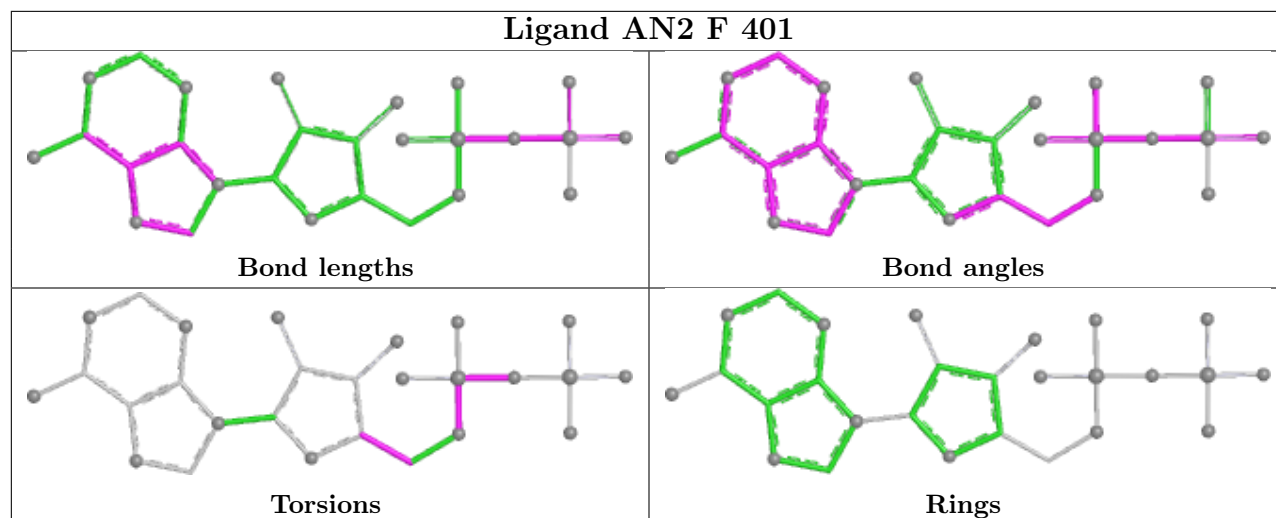
Ligand AN2 J 401



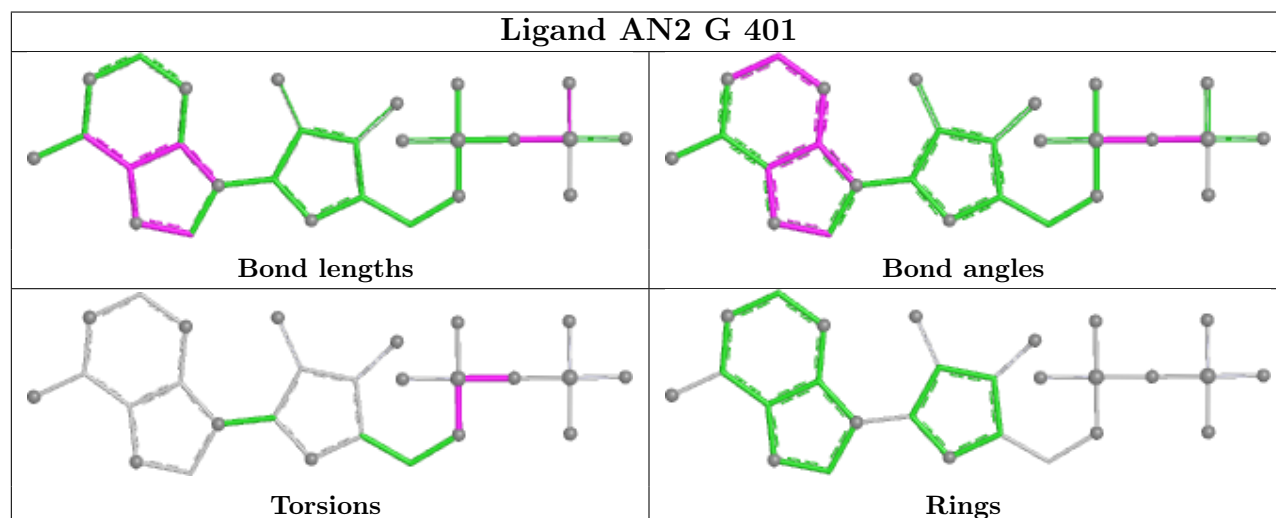
Ligand AN2 L 401



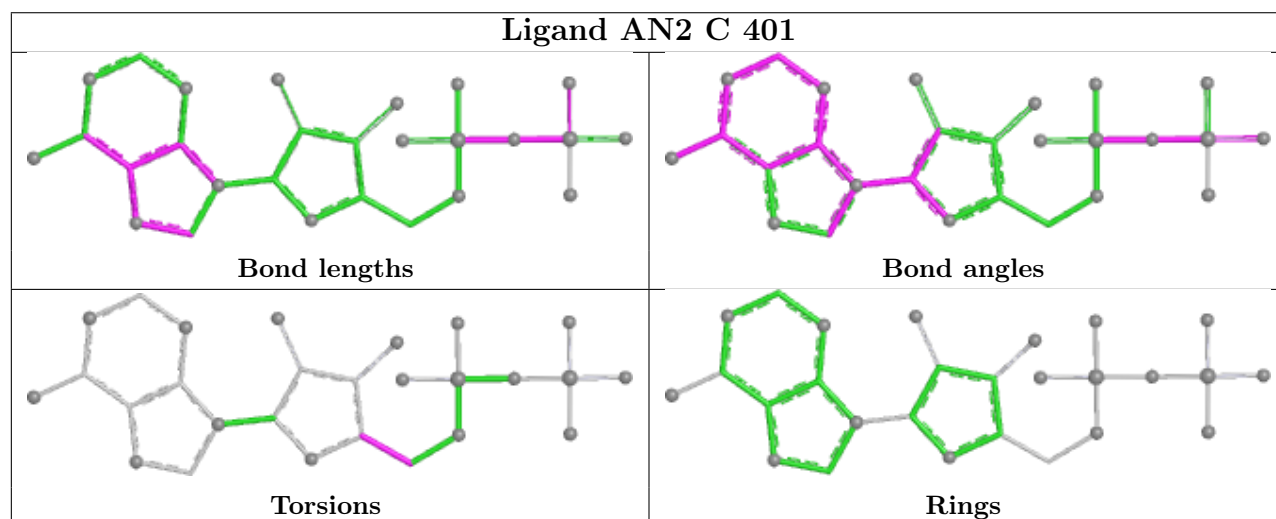
Ligand AN2 F 401



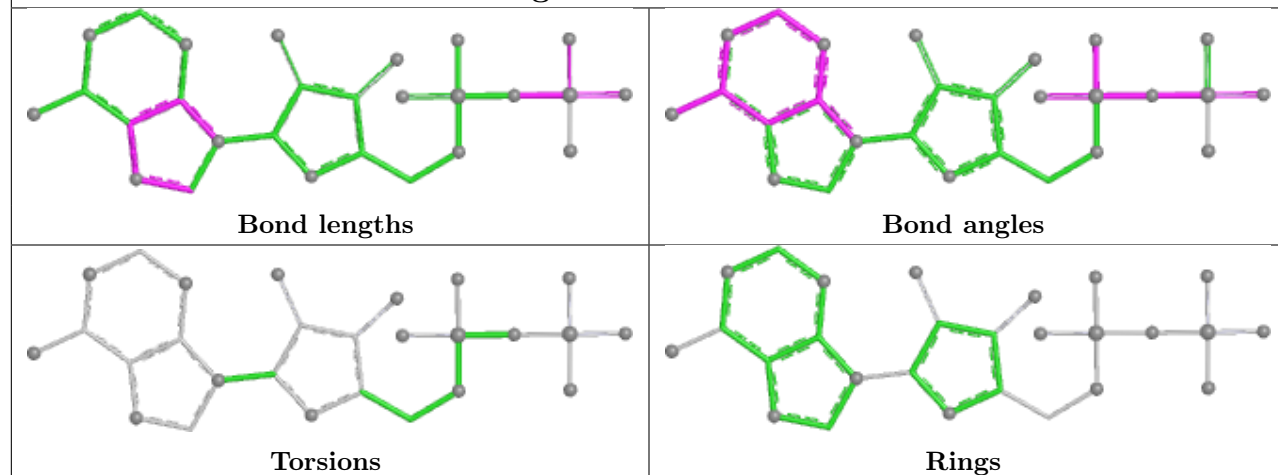
Ligand AN2 G 401



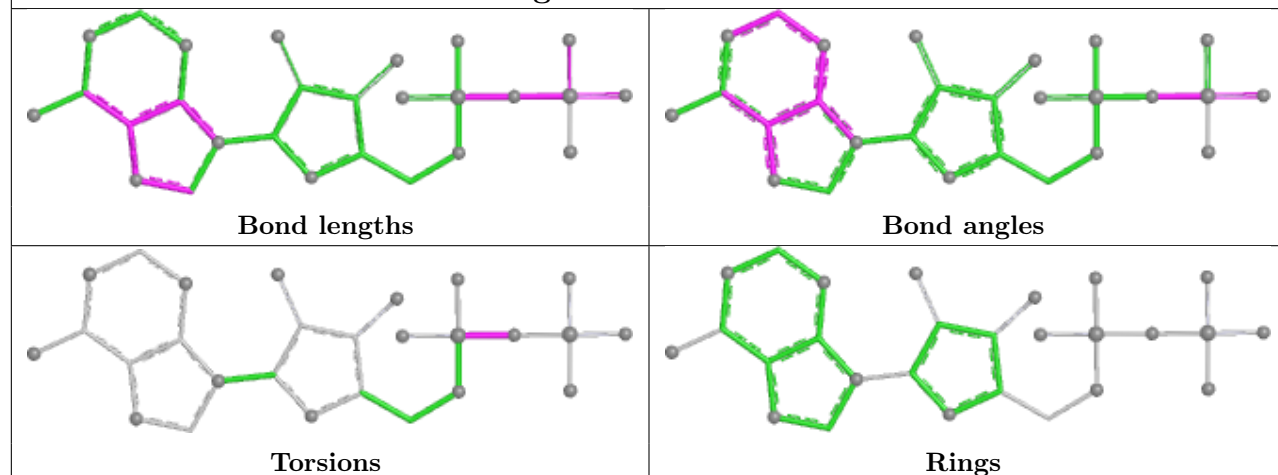
Ligand AN2 C 401



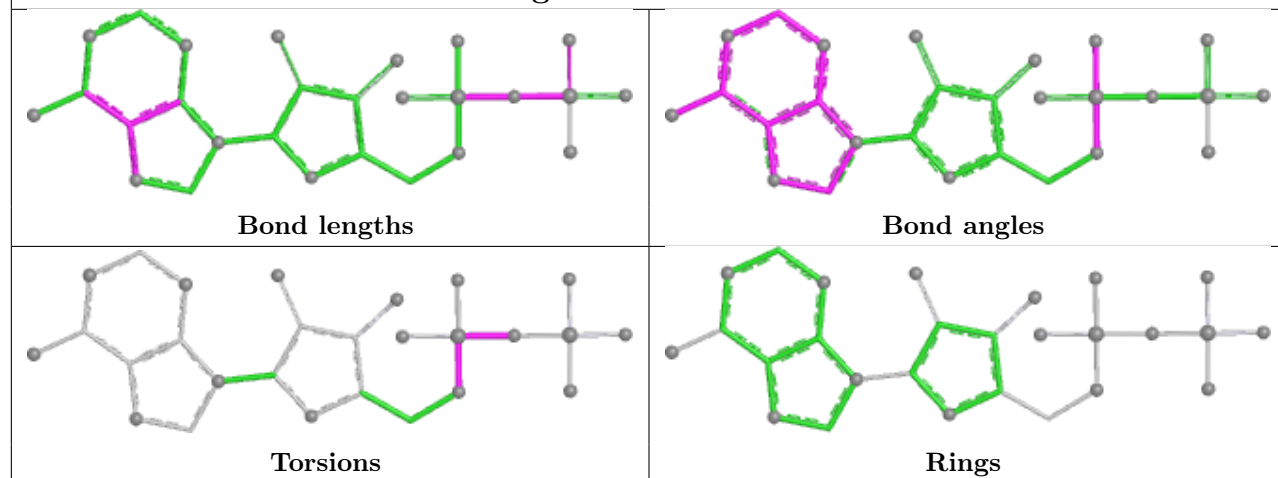
Ligand AN2 H 401

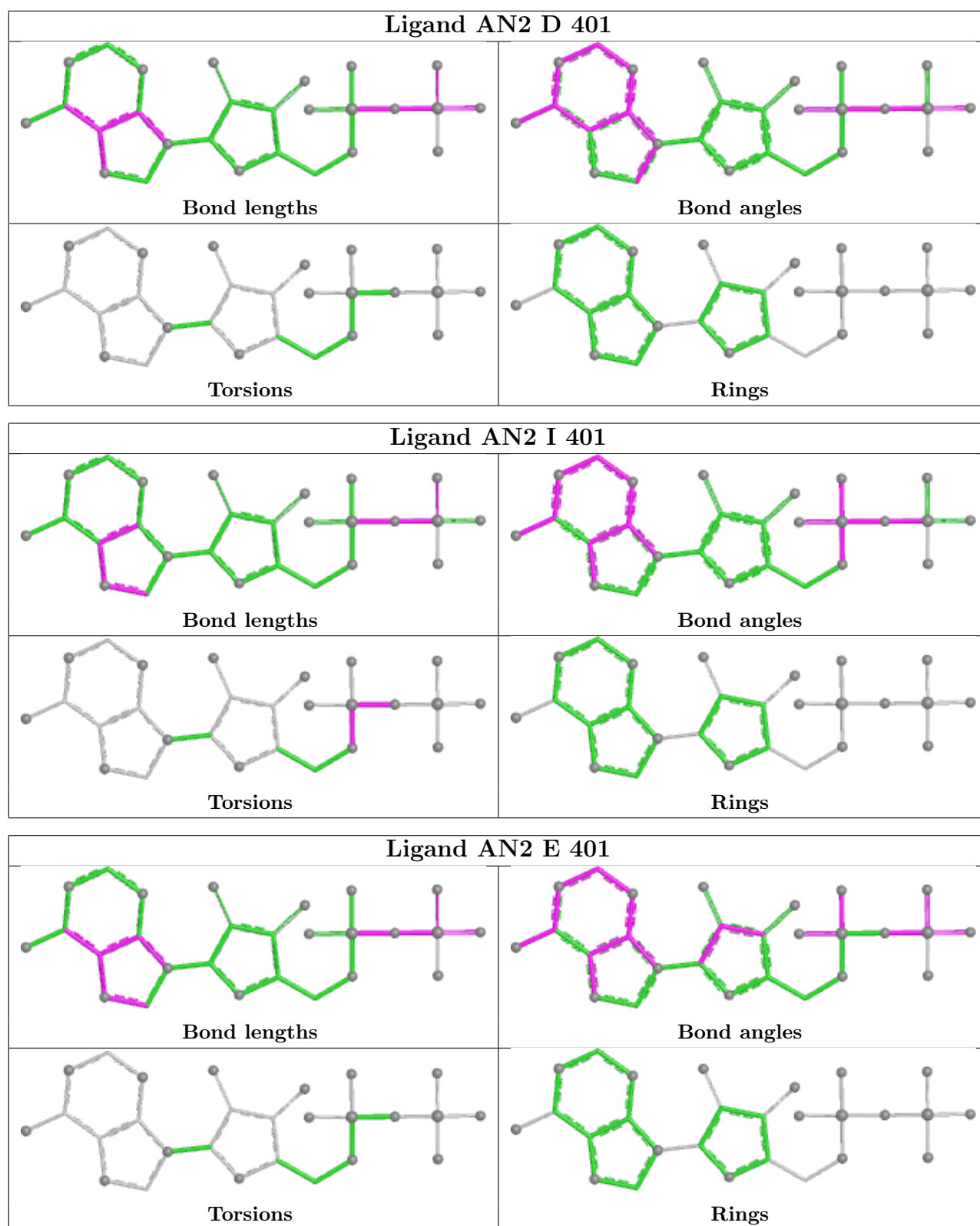


Ligand AN2 B 401



Ligand AN2 K 401





5.7 Other polymers ⓘ

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 [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	306/330 (92%)	-1.19	0 100 100	18, 42, 95, 110	0
1	B	314/330 (95%)	-1.59	0 100 100	17, 33, 62, 84	1 (0%)
1	C	313/330 (94%)	-1.55	0 100 100	10, 33, 64, 80	1 (0%)
1	D	311/330 (94%)	-1.51	0 100 100	15, 34, 59, 77	1 (0%)
1	E	311/330 (94%)	-1.63	0 100 100	14, 29, 54, 75	1 (0%)
1	F	312/330 (94%)	-1.37	0 100 100	22, 44, 81, 93	0
1	G	314/330 (95%)	-1.67	0 100 100	16, 31, 51, 67	0
1	H	311/330 (94%)	-1.64	0 100 100	17, 30, 52, 90	0
1	I	313/330 (94%)	-1.30	0 100 100	24, 43, 88, 121	0
1	J	314/330 (95%)	-1.40	0 100 100	27, 45, 71, 99	0
1	K	312/330 (94%)	-1.41	0 100 100	13, 39, 74, 90	4 (1%)
1	L	311/330 (94%)	-1.39	0 100 100	15, 41, 70, 90	1 (0%)
All	All	3742/3960 (94%)	-1.47	0 100 100	10, 37, 72, 121	9 (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](#)

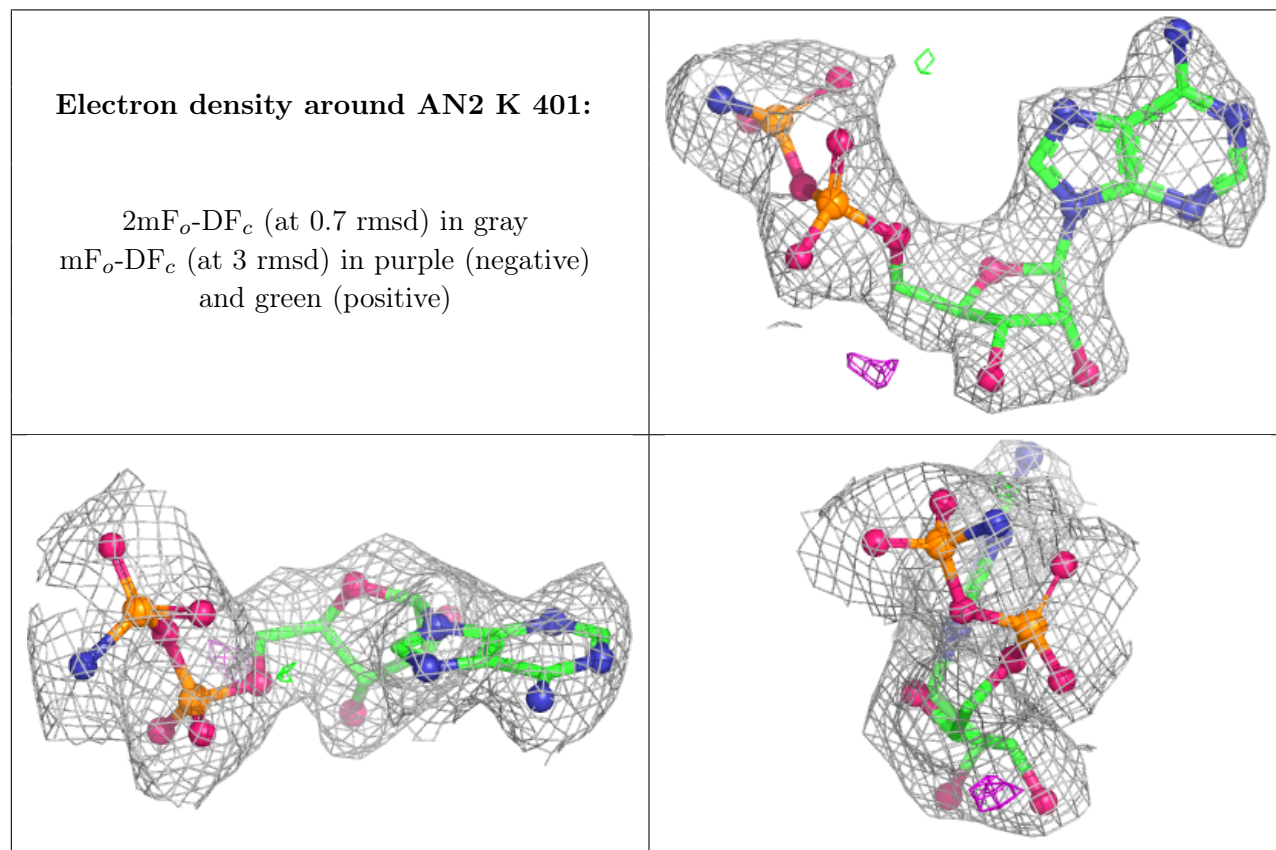
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

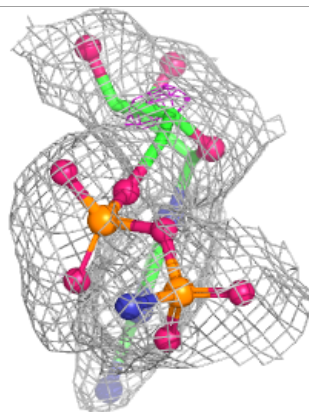
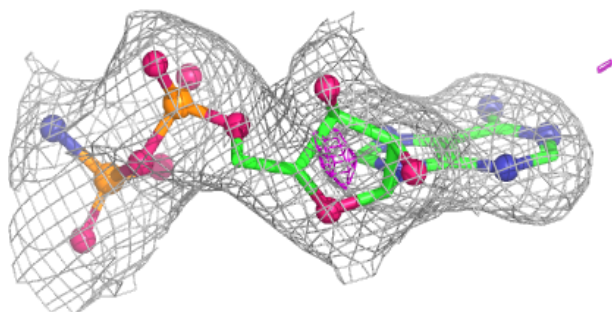
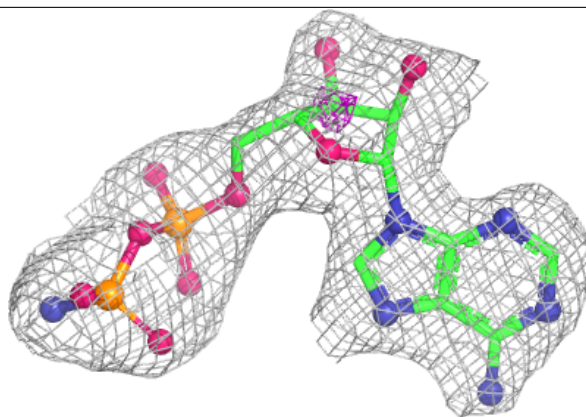
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NA	L	403	1/1	0.98	0.04	47,47,47,47	0
2	AN2	K	401	27/27	0.99	0.03	42,46,60,60	0
2	AN2	L	401	27/27	0.99	0.03	33,37,51,54	0
3	NA	A	402	1/1	0.99	0.03	26,26,26,26	0
3	NA	B	403	1/1	0.99	0.03	31,31,31,31	0
3	NA	C	402	1/1	0.99	0.04	29,29,29,29	0
3	NA	C	403	1/1	0.99	0.03	28,28,28,28	0
3	NA	D	402	1/1	0.99	0.02	26,26,26,26	0
3	NA	D	403	1/1	0.99	0.02	34,34,34,34	0
3	NA	E	402	1/1	0.99	0.04	25,25,25,25	0
3	NA	F	402	1/1	0.99	0.03	50,50,50,50	0
3	NA	F	403	1/1	0.99	0.02	35,35,35,35	0
3	NA	G	403	1/1	0.99	0.03	17,17,17,17	0
3	NA	H	403	1/1	0.99	0.03	21,21,21,21	0
3	NA	I	402	1/1	0.99	0.03	33,33,33,33	0
3	NA	I	403	1/1	0.99	0.03	38,38,38,38	0
3	NA	J	402	1/1	0.99	0.04	38,38,38,38	0
3	NA	L	402	1/1	0.99	0.03	26,26,26,26	0
2	AN2	B	401	27/27	0.99	0.03	26,31,38,40	0
2	AN2	I	401	27/27	1.00	0.02	35,39,48,50	0
2	AN2	J	401	27/27	1.00	0.03	26,36,41,47	0
3	NA	E	403	1/1	1.00	0.05	26,26,26,26	0
2	AN2	A	401	27/27	1.00	0.03	35,45,58,59	0
2	AN2	C	401	27/27	1.00	0.02	29,36,43,43	0
3	NA	G	402	1/1	1.00	0.02	28,28,28,28	0
2	AN2	D	401	27/27	1.00	0.03	29,34,38,38	0
3	NA	H	402	1/1	1.00	0.01	33,33,33,33	0
3	NA	A	403	1/1	1.00	0.02	31,31,31,31	0
3	NA	B	402	1/1	1.00	0.02	22,22,22,22	0
2	AN2	E	401	27/27	1.00	0.02	24,29,37,39	0
2	AN2	F	401	27/27	1.00	0.03	32,48,56,63	0
3	NA	J	403	1/1	1.00	0.01	27,27,27,27	0
3	NA	K	402	1/1	1.00	0.06	40,40,40,40	0
3	NA	K	403	1/1	1.00	0.02	37,37,37,37	0
2	AN2	G	401	27/27	1.00	0.02	24,26,31,34	0
2	AN2	H	401	27/27	1.00	0.02	18,20,29,30	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.

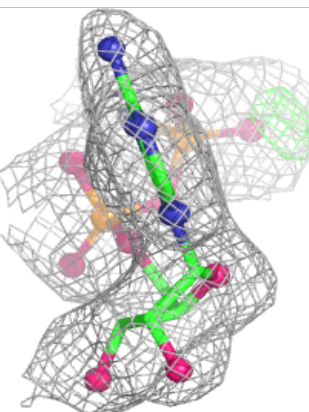
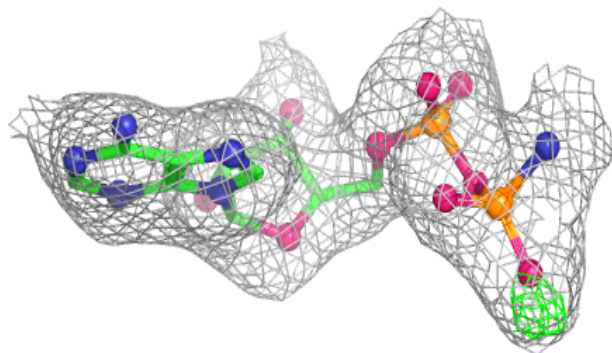
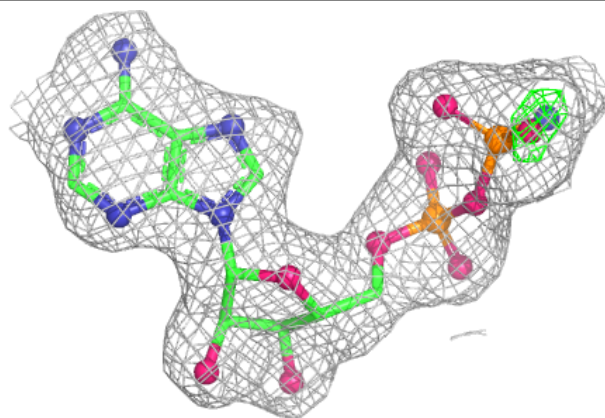


Electron density around AN2 L 401:

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

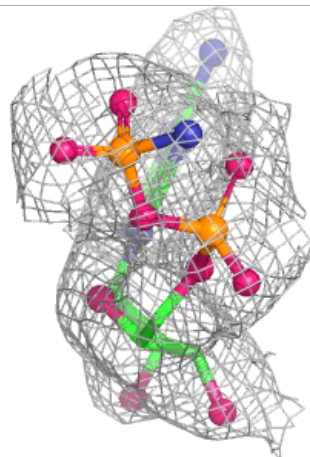
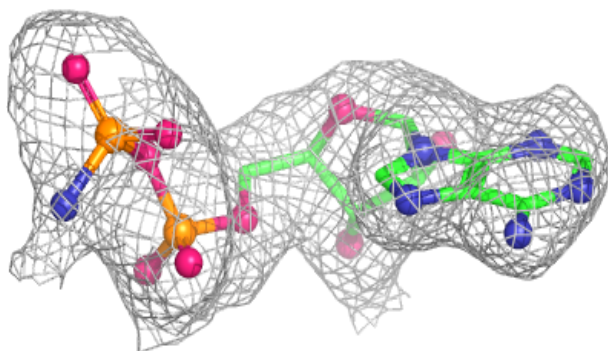
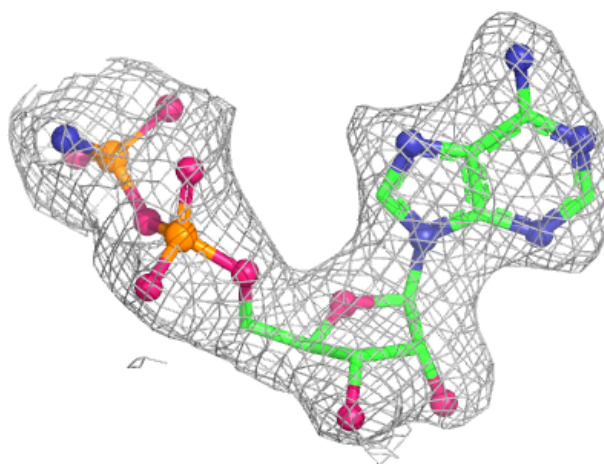
**Electron density around AN2 B 401:**

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



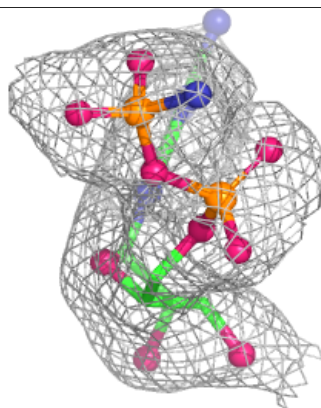
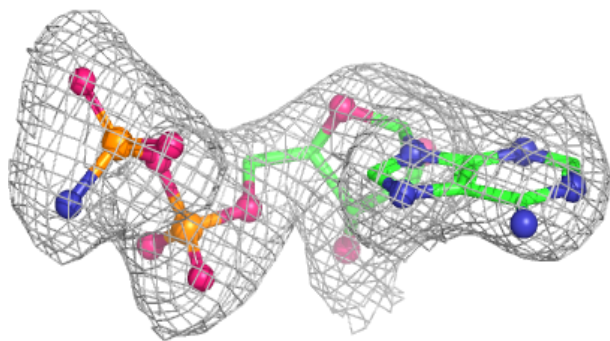
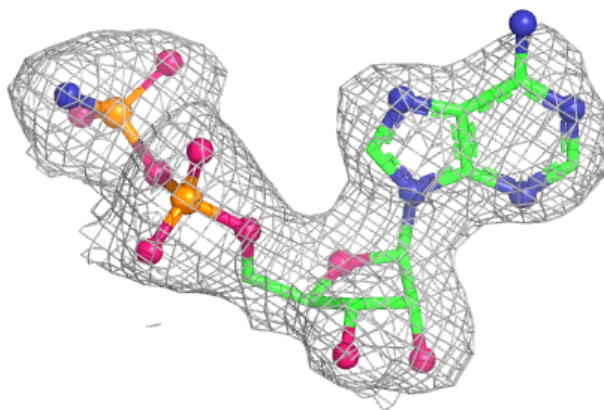
Electron density around AN2 I 401:

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

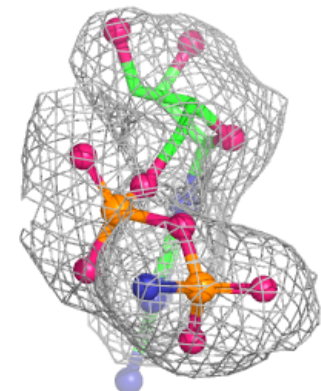
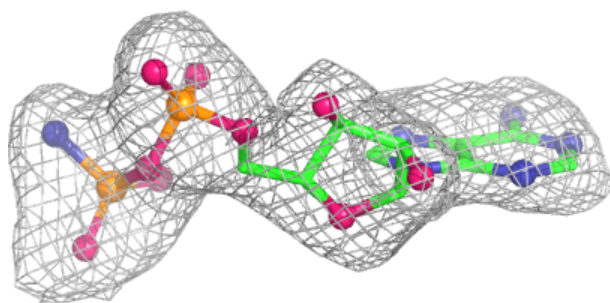
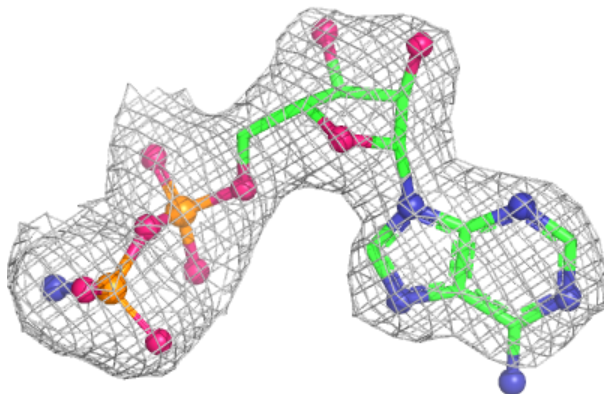


Electron density around AN2 J 401:

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

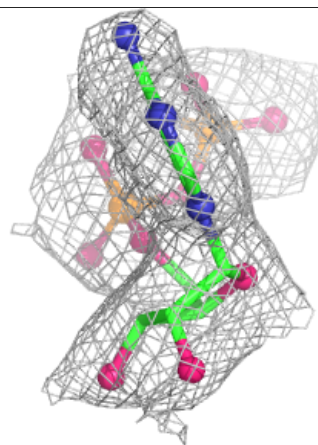
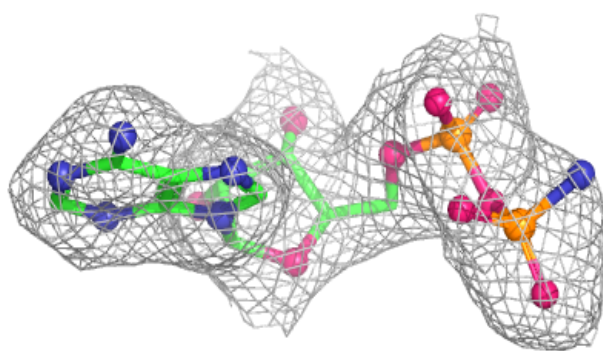
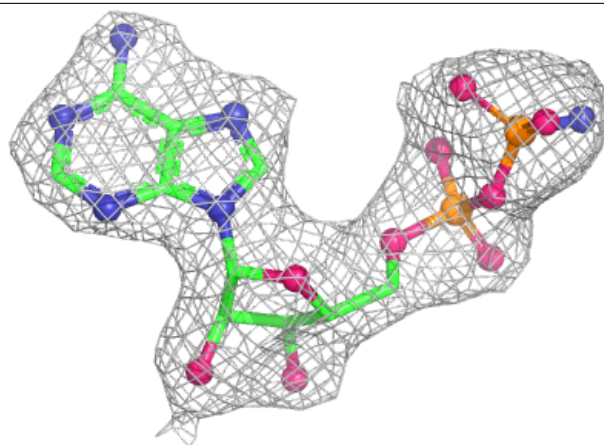
**Electron density around AN2 A 401:**

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



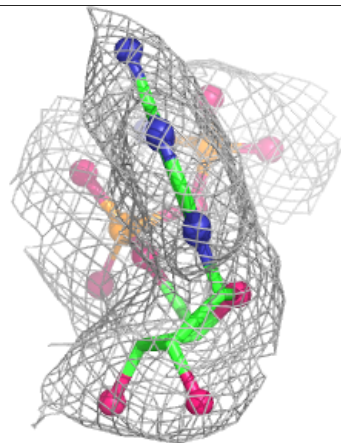
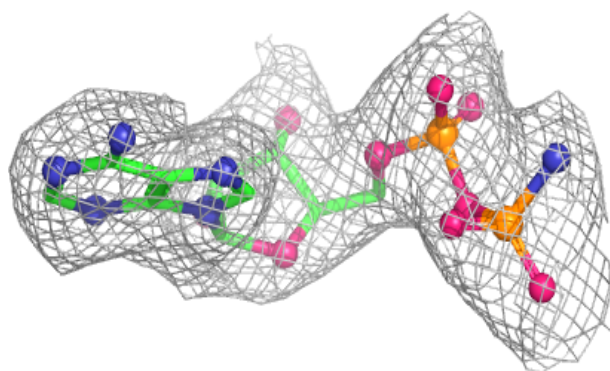
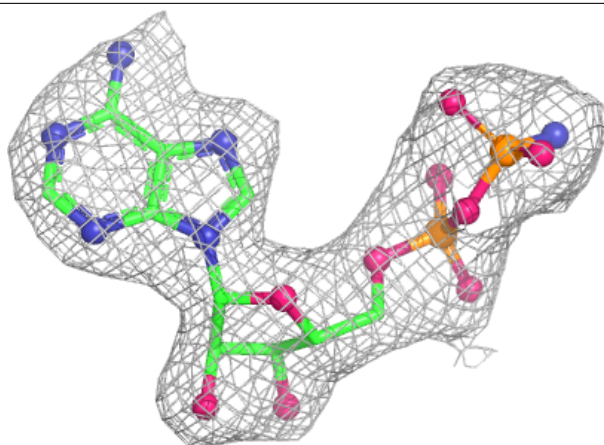
Electron density around AN2 C 401:

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



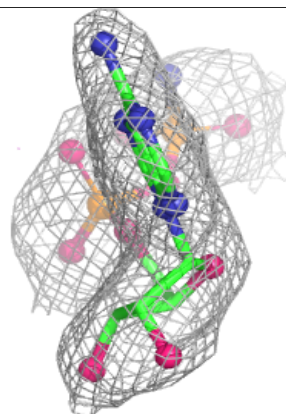
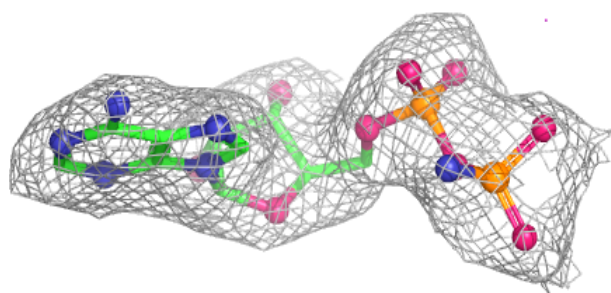
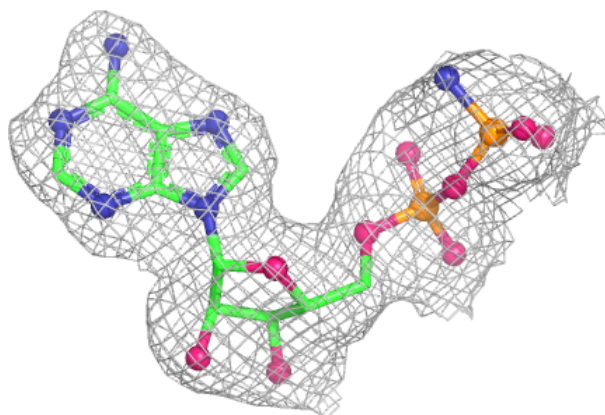
Electron density around AN2 D 401:

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

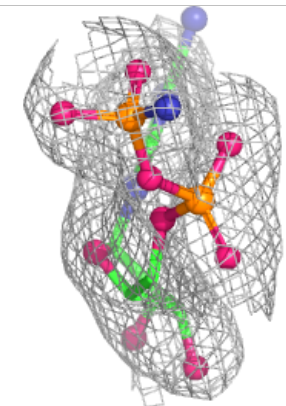
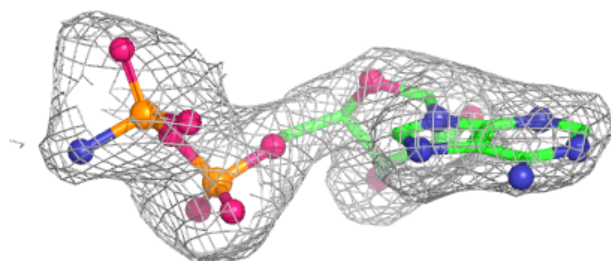
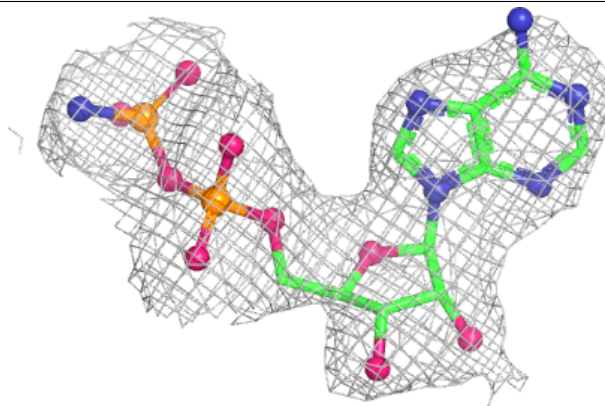


Electron density around AN2 E 401:

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

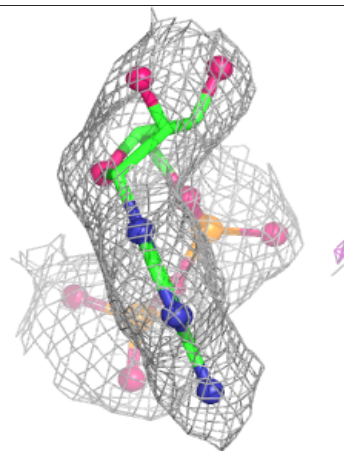
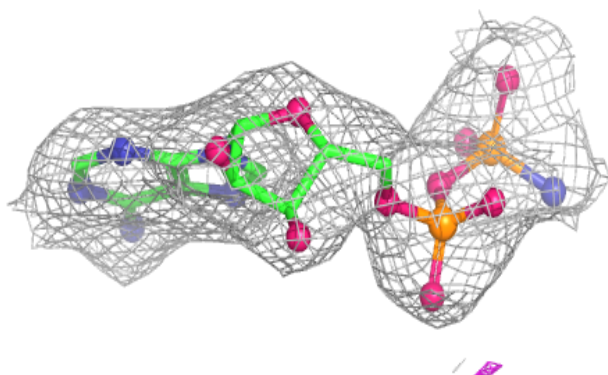
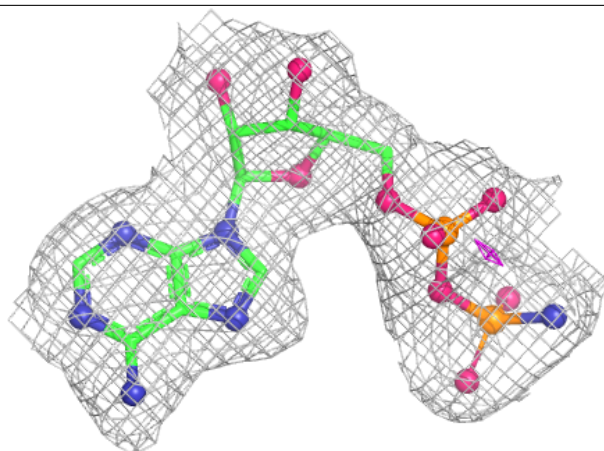
**Electron density around AN2 F 401:**

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

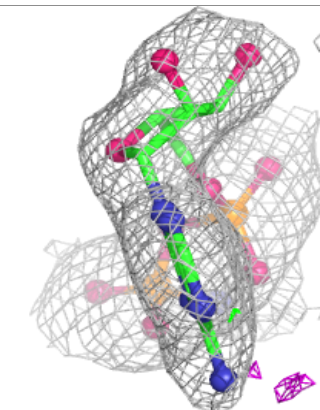
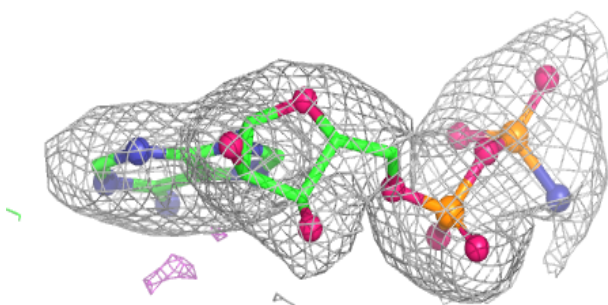
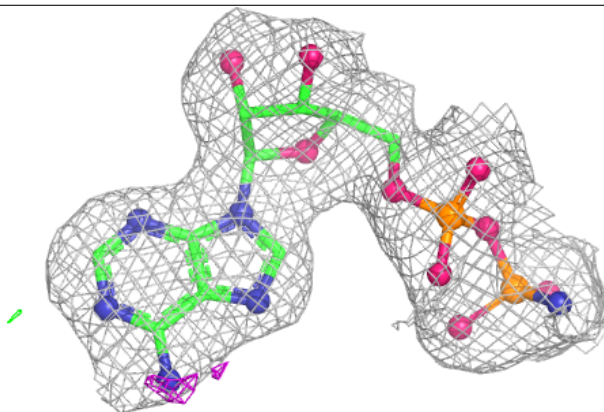


Electron density around AN2 G 401:

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

**Electron density around AN2 H 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.