



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2025 – 01:12 pm BST

PDB ID : 9I1P / pdb_00009i1p
Title : Structure of RecQL- Myc G-quadruplex - ADP complex from Bos taurus
Authors : Song, Z.Y.; Liu, N.N.; Ai, X.; Rety, S.; Xi, X.G.
Deposited on : 2025-01-16
Resolution : 3.20 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:

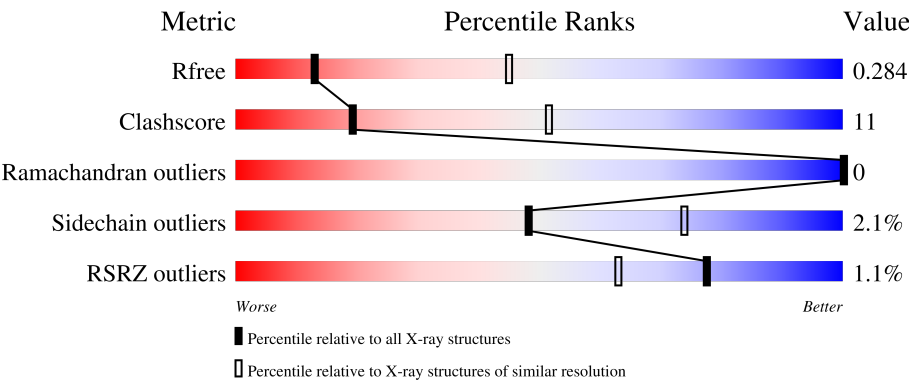
MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.46

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	531	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>73%25%.</div></div>
1	B	531	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>74%25%.</div></div>
1	C	531	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>74%24%..</div></div>
1	D	531	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>72%26%. </div></div>
2	E	24	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>38%46%. 12%</div></div>

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Mol	Chain	Length	Quality of chain
2	F	24	
2	G	24	
2	H	24	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18822 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 ATP-dependent DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	B	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	C	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			
1	D	531	Total	C	N	O	S	0	0	0
			4237	2704	727	770	36			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	MET	-	initiating methionine	UNP A0JN36
B	62	MET	-	initiating methionine	UNP A0JN36
C	62	MET	-	initiating methionine	UNP A0JN36
D	62	MET	-	initiating methionine	UNP A0JN36

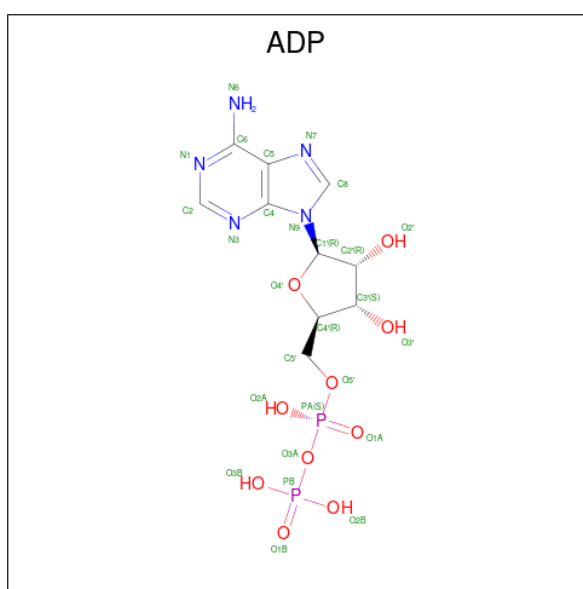
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*GP*GP*TP*GP*GP*GP*TP*A P*GP*GP*GP*TP*GP*GP*GP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	P	0	0	0
			446	210	84	131	21			
2	F	19	Total	C	N	O	P	0	0	0
			405	190	77	119	19			
2	G	21	Total	C	N	O	P	0	0	0
			446	210	84	131	21			
2	H	21	Total	C	N	O	P	0	0	0
			443	210	84	129	20			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 26 10 5 9 2	0	0
4	B	1	Total C N O P 26 10 5 9 2	0	0
4	C	1	Total C N O P 26 10 5 9 2	0	0
4	D	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

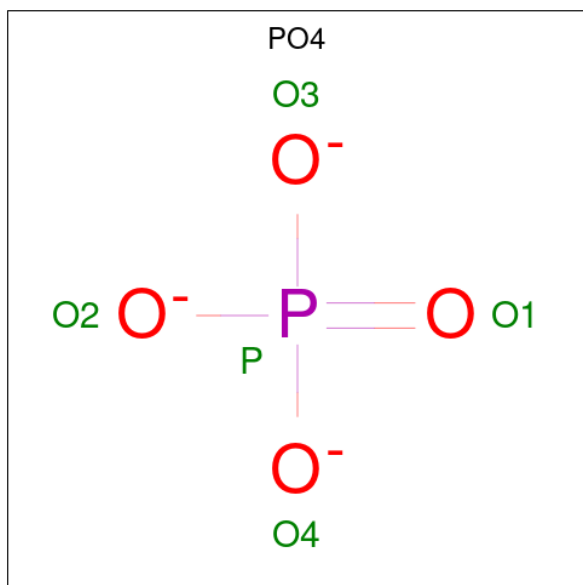
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0

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

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		

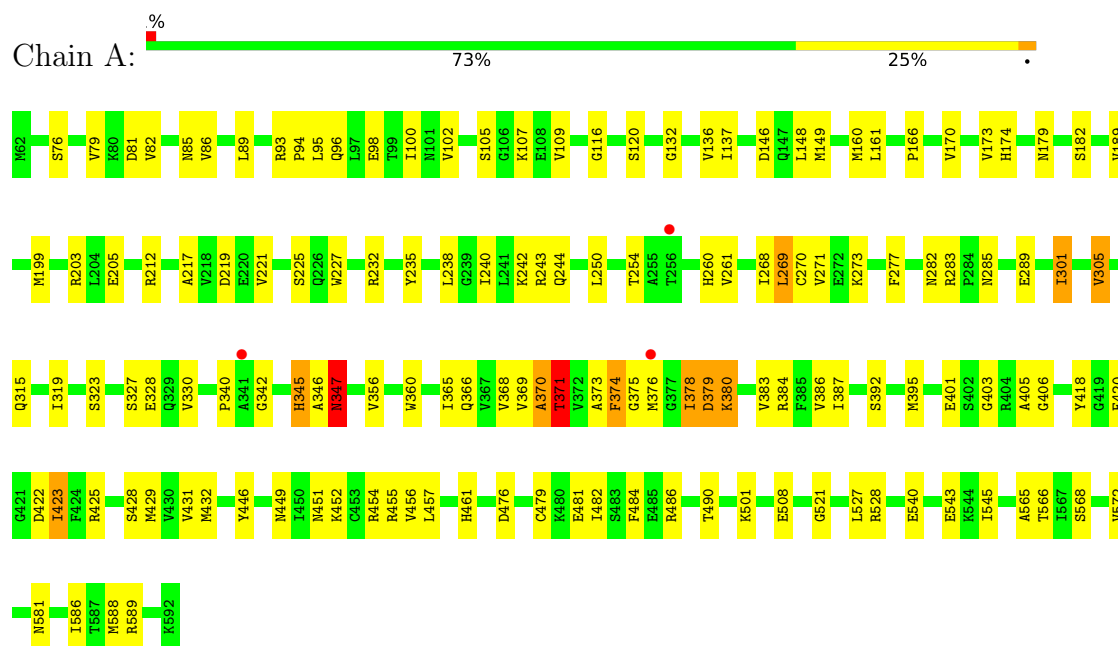
- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	3	Total	K	0	0
			3	3		
7	F	3	Total	K	0	0
			3	3		
7	G	2	Total	K	0	0
			2	2		
7	H	3	Total	K	0	0
			3	3		

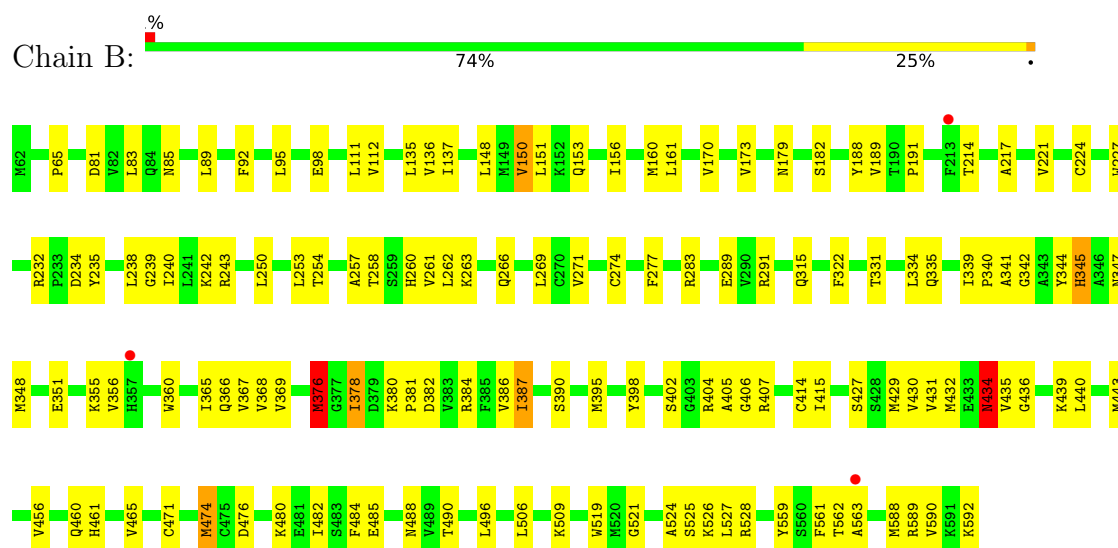
3 Residue-property plots

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

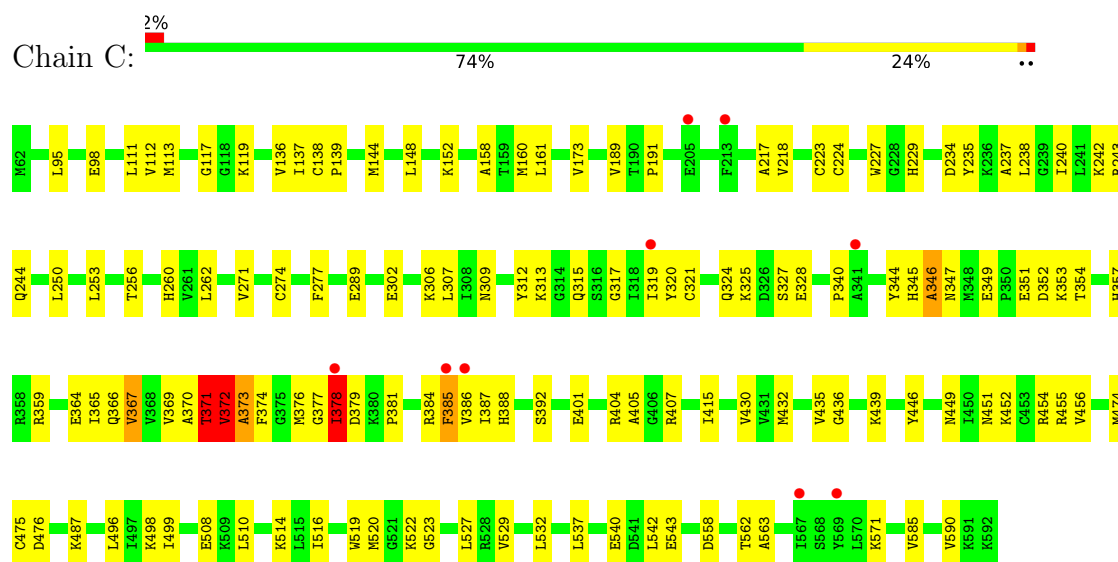
• Molecule 1: ATP-dependent DNA helicase



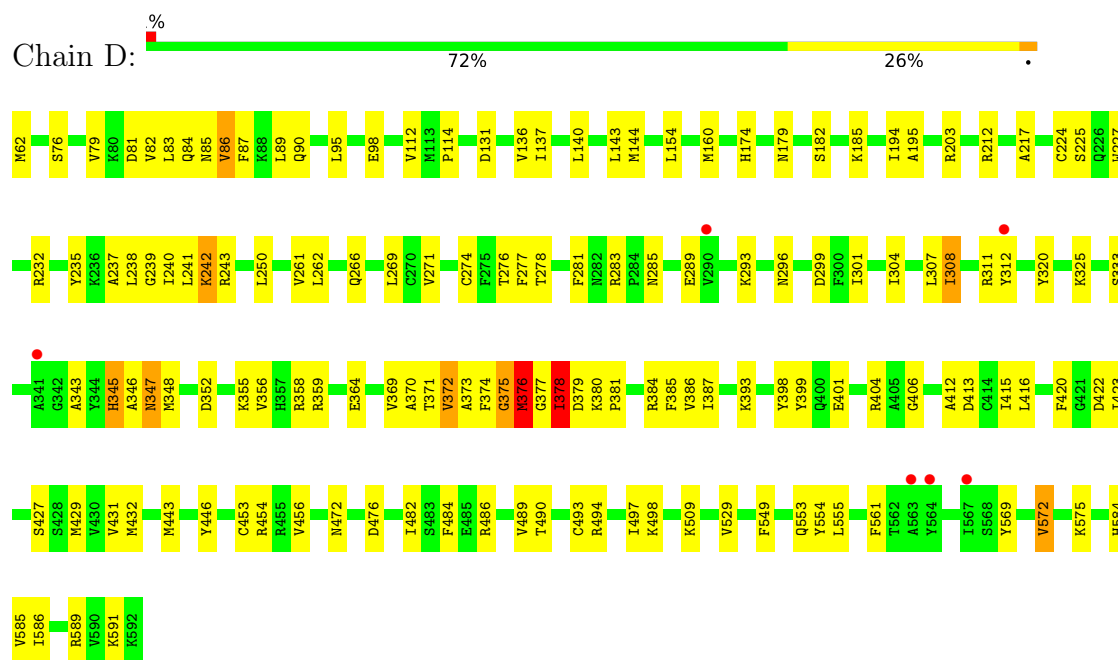
• Molecule 1: ATP-dependent DNA helicase



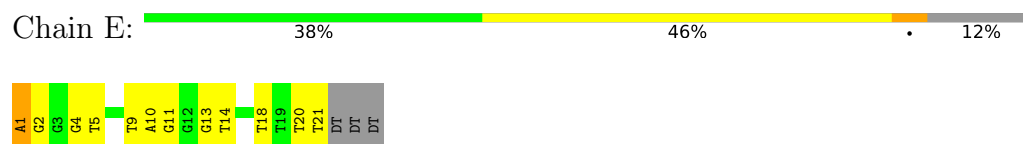
• Molecule 1: ATP-dependent DNA helicase



• Molecule 1: ATP-dependent DNA helicase

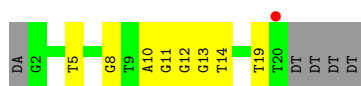


• Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*GP*GP*TP*AP*GP*GP*GP*TP*GP*GP*GP*TP*TP*TP*T)-3')



• Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*GP*GP*TP*AP*GP*GP*GP*TP*GP*GP*GP*TP*TP*TP*T)-3')





- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*GP*GP*TP*AP*GP*GP*GP*TP*GP*GP*GP*TP*TP*TP*T)-3')



- Molecule 2: DNA (5'-D(P*AP*GP*GP*GP*TP*GP*GP*GP*TP*AP*GP*GP*GP*TP*GP*GP*GP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	125.44Å 126.42Å 198.20Å 90.00° 100.90° 90.00°	Depositor
Resolution (Å)	76.55 – 3.20 76.55 – 3.20	Depositor EDS
% Data completeness (in resolution range)	74.7 (76.55-3.20) 75.0 (76.55-3.20)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.244 , 0.288 0.243 , 0.284	Depositor DCC
R_{free} test set	1847 reflections (3.66%)	wwPDB-VP
Wilson B-factor (Å ²)	89.3	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.5	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	0.90	EDS
Total number of atoms	18822	wwPDB-VP
Average B, all atoms (Å ²)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.02% 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: ADP, PO4, ZN, MG, K

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	0.15	0/4325	0.55	9/5830 (0.2%)
1	B	0.13	0/4325	0.44	2/5830 (0.0%)
1	C	0.12	0/4325	0.48	8/5830 (0.1%)
1	D	0.17	0/4325	0.53	9/5830 (0.2%)
2	E	0.27	0/501	0.68	3/776 (0.4%)
2	F	0.22	0/455	0.46	0/705
2	G	0.24	0/501	0.47	0/776
2	H	0.24	0/498	0.49	0/772
All	All	0.15	0/19255	0.51	31/26349 (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	7
1	B	0	4
1	C	0	6
1	D	0	2
All	All	0	19

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	378	ILE	CA-C-N	10.49	143.48	125.02
1	A	378	ILE	C-N-CA	10.49	143.48	125.02
1	D	377	GLY	CA-C-N	10.23	134.94	122.26
1	D	377	GLY	C-N-CA	10.23	134.94	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	DA	OP2-P-O3'	-8.68	81.96	108.00
1	A	371	THR	CA-C-N	8.54	135.54	121.54
1	A	371	THR	C-N-CA	8.54	135.54	121.54
1	D	376	MET	CA-C-N	8.39	137.87	121.41
1	D	376	MET	C-N-CA	8.39	137.87	121.41
2	E	1	DA	OP1-P-O3'	-8.00	84.01	108.00
1	A	379	ASP	CB-CA-C	-7.87	95.30	110.65
1	D	378	ILE	N-CA-C	-7.51	105.22	111.91
1	D	378	ILE	CA-C-N	6.88	130.43	120.38
1	D	378	ILE	C-N-CA	6.88	130.43	120.38
1	C	371	THR	CA-C-N	-6.70	110.31	121.63
1	C	371	THR	C-N-CA	-6.70	110.31	121.63
1	B	434	ASN	CA-C-N	6.59	132.34	121.54
1	B	434	ASN	C-N-CA	6.59	132.34	121.54
1	A	479	CYS	CA-C-N	6.24	132.16	121.86
1	A	479	CYS	C-N-CA	6.24	132.16	121.86
1	C	373	ALA	CA-C-N	-6.23	111.65	122.36
1	C	373	ALA	C-N-CA	-6.23	111.65	122.36
2	E	2	DG	OP1-P-OP2	5.64	136.94	120.00
1	A	370	ALA	CA-C-N	5.48	131.18	122.74
1	A	370	ALA	C-N-CA	5.48	131.18	122.74
1	D	376	MET	N-CA-CB	5.26	119.07	110.55
1	C	372	VAL	CA-C-N	5.20	129.61	121.76
1	C	372	VAL	C-N-CA	5.20	129.61	121.76
1	C	378	ILE	CA-C-N	5.17	129.63	121.56
1	C	378	ILE	C-N-CA	5.17	129.63	121.56
1	D	372	VAL	N-CA-C	-5.14	106.23	112.76

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	LEU	Peptide
1	A	345	HIS	Peptide
1	A	347	ASN	Peptide
1	A	371	THR	Peptide
1	A	375	GLY	Peptide
1	A	380	LYS	Peptide
1	A	482	ILE	Peptide
1	B	347	ASN	Peptide
1	B	376	MET	Peptide
1	B	434	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	B	435	VAL	Peptide
1	C	346	ALA	Peptide
1	C	347	ASN	Peptide
1	C	366	GLN	Peptide
1	C	372	VAL	Peptide
1	C	378	ILE	Peptide
1	C	385	PHE	Peptide
1	D	375	GLY	Peptide
1	D	376	MET	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4237	0	4293	107	0
1	B	4237	0	4295	93	0
1	C	4237	0	4296	103	0
1	D	4237	0	4294	101	0
2	E	446	0	239	19	0
2	F	405	0	216	7	0
2	G	446	0	239	10	0
2	H	443	0	240	8	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	26	0	12	5	0
4	B	26	0	12	0	0
4	C	26	0	12	2	0
4	D	27	0	12	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	B	5	0	0	1	0
6	F	5	0	0	0	0
7	E	3	0	0	0	0
7	F	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	2	0	0	0	0
7	H	3	0	0	0	0
All	All	18822	0	18160	424	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (424) 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:376:MET:HE1	1:C:379:ASP:HA	1.50	0.94
1:B:376:MET:HA	1:B:378:ILE:HG23	1.60	0.83
1:D:311:ARG:NH1	1:D:413:ASP:OD2	2.14	0.78
1:D:81:ASP:OD1	1:D:85:ASN:ND2	2.16	0.78
1:B:289:GLU:HA	1:B:476:ASP:HB2	1.66	0.77
1:C:240:ILE:HD11	1:D:432:MET:HA	1.65	0.77
1:A:105:SER:OG	1:A:107:LYS:NZ	2.18	0.77
1:A:449:ASN:HD22	1:A:457:LEU:HD11	1.50	0.76
1:A:581:ASN:ND2	1:C:451:ASN:O	2.19	0.74
1:C:432:MET:HE2	1:D:195:ALA:HA	1.69	0.74
1:A:120:SER:N	4:A:1002:ADP:O1A	2.20	0.74
1:A:449:ASN:HD21	1:A:452:LYS:HB2	1.52	0.74
1:C:376:MET:HE3	1:C:377:GLY:H	1.54	0.72
1:B:340:PRO:HG2	1:B:366:GLN:H	1.52	0.72
1:C:289:GLU:HA	1:C:476:ASP:HB2	1.70	0.71
1:D:271:VAL:HG22	1:D:274:CYS:HB2	1.73	0.71
1:B:240:ILE:HD12	1:B:243:ARG:HD3	1.71	0.70
1:B:381:PRO:HA	1:B:407:ARG:HB3	1.73	0.70
1:B:506:LEU:HD13	1:B:526:LYS:HE3	1.73	0.70
1:B:376:MET:HA	1:B:378:ILE:H	1.54	0.70
1:B:431:VAL:HG11	1:B:559:TYR:CZ	2.26	0.69
1:D:376:MET:C	1:D:378:ILE:HG12	2.18	0.69
1:B:235:TYR:HA	1:B:238:LEU:HD13	1.74	0.69
1:C:449:ASN:HD21	1:C:452:LYS:HE3	1.57	0.69
1:A:232:ARG:HB2	1:A:235:TYR:HB2	1.74	0.68
1:A:340:PRO:HB2	1:A:365:ILE:HA	1.75	0.68
1:A:386:VAL:HG23	1:A:405:ALA:HB2	1.74	0.67
1:A:374:PHE:H	1:A:374:PHE:HD2	1.39	0.67
1:A:347:ASN:O	1:A:347:ASN:ND2	2.24	0.67
1:A:161:LEU:HD11	1:A:173:VAL:HG11	1.75	0.66
1:A:451:ASN:HB3	1:A:484:PHE:HE2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:ASN:O	1:D:347:ASN:ND2	2.28	0.66
1:D:232:ARG:HB2	1:D:235:TYR:HD2	1.60	0.66
1:B:386:VAL:HG23	1:B:405:ALA:HB2	1.78	0.66
1:A:370:ALA:HB3	1:A:374:PHE:CZ	2.31	0.65
1:A:179:ASN:O	1:A:212:ARG:NH1	2.30	0.65
1:C:119:LYS:NZ	4:C:1002:ADP:O3B	2.29	0.65
1:D:373:ALA:O	1:D:374:PHE:C	2.40	0.65
1:D:179:ASN:O	1:D:212:ARG:NH1	2.29	0.65
1:D:446:TYR:O	1:D:454:ARG:NH1	2.29	0.65
1:C:454:ARG:HE	1:C:476:ASP:HB3	1.60	0.64
1:A:451:ASN:HB3	1:A:484:PHE:CE2	2.32	0.64
1:B:398:TYR:HB2	1:B:443:MET:HE1	1.80	0.63
1:C:381:PRO:HA	1:C:407:ARG:HB3	1.80	0.63
1:D:182:SER:HB3	1:D:212:ARG:HH12	1.63	0.63
1:A:360:TRP:CZ3	1:A:380:LYS:HG2	2.34	0.63
1:D:379:ASP:HB3	4:D:1002:ADP:O3'	1.99	0.63
1:B:271:VAL:HG22	1:B:274:CYS:HB2	1.81	0.63
2:E:10:DA:C8	2:E:10:DA:H5''	2.34	0.62
1:B:484:PHE:HD1	1:B:592:LYS:HB2	1.65	0.62
1:B:81:ASP:OD1	1:B:85:ASN:ND2	2.25	0.62
1:B:378:ILE:HG12	1:B:404:ARG:HD3	1.79	0.62
1:D:242:LYS:HE3	1:D:271:VAL:HB	1.81	0.62
1:C:271:VAL:HG22	1:C:274:CYS:HB2	1.80	0.62
1:C:95:LEU:HD13	1:C:277:PHE:HB3	1.80	0.62
1:C:432:MET:HE3	1:D:237:ALA:HB1	1.81	0.62
1:A:102:VAL:HG13	1:A:107:LYS:HE2	1.82	0.62
1:C:319:ILE:HB	1:C:369:VAL:HG12	1.82	0.61
1:B:242:LYS:HZ1	1:B:250:LEU:HD22	1.66	0.61
1:D:355:LYS:HA	1:D:358:ARG:HG2	1.81	0.61
1:C:319:ILE:HG12	1:C:387:ILE:HG13	1.81	0.60
1:C:317:GLY:HA3	1:C:385:PHE:HB2	1.82	0.60
1:A:76:SER:HA	1:A:79:VAL:HG22	1.83	0.60
1:A:219:ASP:O	1:A:235:TYR:OH	2.19	0.60
1:A:240:ILE:HD12	1:A:243:ARG:HD3	1.84	0.60
1:B:589:ARG:NH2	6:B:1004:PO4:O3	2.26	0.59
1:A:95:LEU:HD13	1:A:277:PHE:HB3	1.83	0.59
1:C:320:TYR:HB2	1:C:388:HIS:ND1	2.16	0.59
1:B:291:ARG:HD2	1:B:415:ILE:HD11	1.84	0.59
1:C:499:ILE:HG22	1:C:529:VAL:HG23	1.83	0.59
1:C:237:ALA:O	1:C:240:ILE:HD12	2.03	0.59
1:D:83:LEU:HD11	1:D:89:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:PRO:HB2	1:B:365:ILE:HA	1.84	0.59
1:D:311:ARG:NH2	1:D:312:TYR:OH	2.35	0.59
1:B:480:LYS:HG2	1:B:482:ILE:HG12	1.85	0.59
1:A:346:ALA:HB2	2:E:20:DT:P	2.43	0.58
1:A:161:LEU:HB2	1:A:189:VAL:HG12	1.86	0.58
1:B:342:GLY:HA3	1:B:368:VAL:HA	1.86	0.58
1:B:345:HIS:CE1	1:B:348:MET:HB2	2.39	0.58
1:A:242:LYS:HE2	1:A:271:VAL:HG22	1.86	0.57
1:B:137:ILE:HG21	1:B:238:LEU:HD21	1.85	0.57
1:B:429:MET:HB3	2:F:19:DT:H3	1.70	0.57
1:B:232:ARG:HB2	1:B:235:TYR:HD2	1.69	0.57
1:D:242:LYS:HE2	1:D:269:LEU:O	2.04	0.57
1:C:435:VAL:HG23	1:C:439:LYS:HE2	1.87	0.57
1:D:346:ALA:HB2	2:H:20:DT:OP2	2.05	0.57
1:A:373:ALA:HB2	2:E:20:DT:H4'	1.86	0.57
1:A:486:ARG:HH21	1:A:589:ARG:HH21	1.50	0.57
1:A:242:LYS:HD3	1:A:250:LEU:HD13	1.85	0.57
1:A:379:ASP:CG	4:A:1002:ADP:H4'	2.29	0.57
1:A:521:GLY:O	1:A:528:ARG:NH2	2.38	0.57
1:D:429:MET:HA	1:D:429:MET:HE2	1.86	0.57
1:C:346:ALA:HA	1:C:353:LYS:HE2	1.85	0.57
1:D:486:ARG:HH21	1:D:589:ARG:HH21	1.53	0.57
1:B:331:THR:HG23	1:B:341:ALA:HB1	1.86	0.56
1:D:420:PHE:O	1:D:423:ILE:HG22	2.05	0.56
1:D:384:ARG:HH21	1:D:412:ALA:HB2	1.68	0.56
1:D:301:ILE:HD13	1:D:304:ILE:HD12	1.88	0.56
1:B:521:GLY:O	1:B:528:ARG:NH2	2.35	0.56
1:D:494:ARG:O	1:D:498:LYS:HD3	2.06	0.56
2:E:1:DA:H5''	2:E:1:DA:H8	1.71	0.56
2:E:9:DT:H2''	2:E:10:DA:H5'	1.86	0.56
1:D:95:LEU:HD13	1:D:277:PHE:HB3	1.87	0.55
1:A:148:LEU:HD11	1:A:160:MET:HB3	1.87	0.55
1:A:330:VAL:HB	1:A:369:VAL:HG11	1.88	0.55
1:B:95:LEU:HD13	1:B:277:PHE:HB3	1.88	0.55
1:C:152:LYS:NZ	1:C:158:ALA:O	2.31	0.55
1:A:418:TYR:CE1	1:A:423:ILE:HD11	2.42	0.55
1:A:137:ILE:HG21	1:A:238:LEU:HD11	1.88	0.55
1:C:455:ARG:NH2	1:C:474:MET:O	2.39	0.55
1:B:239:GLY:HA2	1:B:269:LEU:HA	1.88	0.55
1:C:137:ILE:HD13	1:C:218:VAL:HG22	1.89	0.55
1:B:524:ALA:HB3	1:B:527:LEU:HD13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:LEU:HB2	1:D:143:LEU:HG	1.89	0.54
1:D:232:ARG:HB2	1:D:235:TYR:CD2	2.41	0.54
1:D:371:THR:C	1:D:373:ALA:H	2.14	0.54
1:C:111:LEU:HB3	1:C:253:LEU:HD23	1.90	0.54
1:C:144:MET:HE3	1:C:160:MET:HB2	1.89	0.54
1:B:161:LEU:HB2	1:B:189:VAL:HG12	1.88	0.54
1:C:242:LYS:HE3	1:C:250:LEU:HB3	1.89	0.54
1:C:302:GLU:O	1:C:306:LYS:HG2	2.08	0.54
1:A:327:SER:HB2	1:A:371:THR:HG23	1.90	0.54
1:B:335:GLN:CG	1:B:341:ALA:HB2	2.37	0.54
1:A:315:GLN:HB3	1:A:384:ARG:HG3	1.89	0.54
1:B:83:LEU:HD11	1:B:89:LEU:HD11	1.89	0.54
1:C:191:PRO:HB2	1:C:234:ASP:HB3	1.89	0.53
1:D:131:ASP:O	1:D:185:LYS:NZ	2.41	0.53
1:D:137:ILE:HG21	1:D:238:LEU:HD11	1.90	0.53
2:F:13:DG:H2''	2:F:14:DT:OP2	2.08	0.53
1:A:102:VAL:HG11	1:A:109:VAL:HB	1.89	0.53
1:B:148:LEU:HD23	1:B:151:LEU:HD12	1.91	0.53
1:A:446:TYR:O	1:A:454:ARG:NH1	2.42	0.53
1:D:62:MET:HE1	1:D:278:THR:HB	1.90	0.53
2:E:10:DA:N3	2:E:10:DA:H2'	2.24	0.53
1:B:111:LEU:HB3	1:B:253:LEU:HD23	1.90	0.53
1:B:161:LEU:HD11	1:B:173:VAL:HG21	1.90	0.53
1:C:387:ILE:HG22	1:C:415:ILE:HB	1.90	0.53
1:C:392:SER:OG	1:C:401:GLU:OE1	2.27	0.53
1:C:317:GLY:HA3	1:C:385:PHE:CD2	2.44	0.53
1:C:558:ASP:HB2	1:C:571:LYS:HE2	1.91	0.52
1:A:161:LEU:HD11	1:A:173:VAL:HG21	1.91	0.52
1:A:379:ASP:OD1	4:A:1002:ADP:H4'	2.09	0.52
1:A:319:ILE:HB	1:A:369:VAL:HG22	1.92	0.52
1:C:98:GLU:OE1	1:C:98:GLU:N	2.42	0.52
1:C:510:LEU:HD21	1:C:527:LEU:HD22	1.91	0.52
1:C:324:GLN:HA	1:C:371:THR:HG21	1.91	0.52
1:A:227:TRP:HZ3	1:A:260:HIS:HB2	1.74	0.52
1:A:323:SER:C	1:A:371:THR:HG21	2.35	0.52
1:A:418:TYR:HE1	1:A:423:ILE:HD11	1.75	0.52
1:B:257:ALA:HB1	1:B:465:VAL:HG11	1.92	0.52
1:D:112:VAL:HG21	1:D:262:LEU:HD21	1.91	0.52
1:B:378:ILE:HG13	1:B:378:ILE:O	2.07	0.52
1:A:501:LYS:HE3	1:A:572:VAL:HG21	1.91	0.51
1:B:484:PHE:HA	1:B:592:LYS:HE3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:GLU:OE1	1:D:98:GLU:N	2.40	0.51
1:D:371:THR:C	1:D:373:ALA:N	2.66	0.51
1:D:398:TYR:HB2	1:D:443:MET:HE1	1.92	0.51
1:C:148:LEU:HD11	1:C:160:MET:HB3	1.92	0.51
1:B:112:VAL:HG21	1:B:262:LEU:HD21	1.92	0.51
2:E:5:DT:C6	2:E:5:DT:H5''	2.45	0.51
1:B:380:LYS:NZ	1:B:382:ASP:OD1	2.44	0.51
1:A:242:LYS:HZ1	1:A:270:CYS:C	2.18	0.51
1:A:379:ASP:O	1:A:380:LYS:C	2.54	0.51
1:D:82:VAL:HA	1:D:86:VAL:HG23	1.93	0.51
1:D:283:ARG:NH2	1:D:406:GLY:O	2.44	0.51
1:D:325:LYS:HE3	2:H:17:DG:OP1	2.11	0.51
2:G:13:DG:H2''	2:G:14:DT:OP2	2.11	0.51
1:D:242:LYS:HD3	1:D:250:LEU:HD13	1.92	0.50
1:D:378:ILE:O	1:D:378:ILE:HG22	2.12	0.50
1:D:398:TYR:CE1	1:D:416:LEU:HD12	2.46	0.50
1:C:357:HIS:NE2	1:C:378:ILE:HG13	2.26	0.50
1:C:317:GLY:HA3	1:C:385:PHE:HD2	1.76	0.50
1:C:487:LYS:HE2	1:C:590:VAL:HG11	1.92	0.50
1:D:242:LYS:HZ3	1:D:250:LEU:HD13	1.76	0.50
1:C:317:GLY:C	1:C:367:VAL:HB	2.36	0.50
1:B:427:SER:O	1:B:431:VAL:HG13	2.12	0.50
1:C:319:ILE:HG12	1:C:387:ILE:CG1	2.41	0.50
1:A:508:GLU:HG2	1:A:527:LEU:HD21	1.94	0.50
1:B:322:PHE:HB2	1:B:390:SER:HB2	1.94	0.50
1:B:334:LEU:HB3	1:B:339:ILE:HB	1.94	0.50
1:D:553:GLN:HB2	1:D:575:LYS:HD3	1.94	0.50
1:C:475:CYS:SG	1:C:476:ASP:N	2.84	0.49
1:D:144:MET:HE3	1:D:160:MET:HB2	1.94	0.49
1:D:453:CYS:O	1:D:456:VAL:HG12	2.12	0.49
2:E:13:DG:H2''	2:E:14:DT:OP2	2.12	0.49
1:A:449:ASN:ND2	1:A:452:LYS:HB2	2.24	0.49
1:C:161:LEU:HD11	1:C:173:VAL:HG21	1.94	0.49
1:C:227:TRP:HZ3	1:C:260:HIS:HB2	1.76	0.49
1:C:349:GLU:HB3	1:C:352:ASP:H	1.78	0.49
2:H:13:DG:H2''	2:H:14:DT:OP2	2.13	0.49
1:A:368:VAL:HG11	1:A:376:MET:HE1	1.95	0.49
1:A:420:PHE:CG	1:A:543:GLU:HB2	2.46	0.49
1:A:428:SER:OG	1:A:568:SER:OG	2.31	0.49
1:A:490:THR:HG23	1:A:586:ILE:H	1.76	0.49
1:B:136:VAL:HA	1:B:217:ALA:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:SER:O	1:A:371:THR:HG21	2.12	0.49
1:A:540:GLU:O	1:A:543:GLU:HG2	2.13	0.49
1:A:301:ILE:O	1:A:305:VAL:HG23	2.13	0.49
1:B:429:MET:HA	1:B:429:MET:HE2	1.94	0.49
1:B:224:CYS:HA	1:B:235:TYR:HB3	1.95	0.48
1:C:112:VAL:HG21	1:C:262:LEU:HD21	1.94	0.48
1:C:376:MET:HE2	1:C:404:ARG:CZ	2.43	0.48
1:C:562:THR:OG1	1:C:563:ALA:N	2.46	0.48
1:B:221:VAL:HG12	1:B:254:THR:HB	1.95	0.48
1:C:315:GLN:HE22	1:C:384:ARG:NH1	2.11	0.48
2:E:9:DT:H2''	2:E:10:DA:C5'	2.43	0.48
1:C:357:HIS:CD2	1:C:378:ILE:HG21	2.48	0.48
2:F:12:DG:H4'	2:F:13:DG:OP1	2.14	0.48
1:A:431:VAL:O	1:A:432:MET:HE2	2.14	0.48
2:E:20:DT:H3'	2:E:21:DT:H5''	1.95	0.48
1:B:315:GLN:HG3	1:B:384:ARG:HG3	1.95	0.48
1:B:387:ILE:HA	1:B:415:ILE:HG23	1.95	0.48
1:C:376:MET:HE1	1:C:379:ASP:CA	2.35	0.48
1:C:496:LEU:HD21	1:C:519:TRP:CE3	2.49	0.48
1:A:370:ALA:HB3	1:A:374:PHE:CE1	2.48	0.48
1:B:179:ASN:HB3	1:B:182:SER:HB2	1.96	0.48
1:A:380:LYS:O	1:A:383:VAL:HG23	2.14	0.47
1:B:148:LEU:HD11	1:B:160:MET:HB3	1.96	0.47
1:C:371:THR:O	1:C:373:ALA:N	2.47	0.47
1:A:81:ASP:OD1	1:A:85:ASN:ND2	2.47	0.47
1:A:98:GLU:OE1	1:A:98:GLU:N	2.44	0.47
1:C:379:ASP:N	1:C:379:ASP:OD1	2.47	0.47
2:H:5:DT:H5''	2:H:5:DT:C6	2.48	0.47
1:B:315:GLN:HG3	1:B:384:ARG:HB2	1.95	0.47
1:B:525:SER:HA	1:B:528:ARG:HH11	1.78	0.47
1:C:240:ILE:HA	1:C:243:ARG:HB2	1.96	0.47
1:C:357:HIS:CD2	1:C:378:ILE:HG13	2.50	0.47
1:D:239:GLY:HA2	1:D:269:LEU:HA	1.95	0.47
1:D:359:ARG:O	1:D:364:GLU:N	2.48	0.47
2:E:10:DA:H2''	2:E:11:DG:OP2	2.15	0.47
2:G:5:DT:C6	2:G:5:DT:H5''	2.49	0.47
1:A:82:VAL:O	1:A:86:VAL:HG22	2.15	0.47
1:D:174:HIS:ND1	1:D:203:ARG:HG3	2.30	0.47
2:H:13:DG:H4'	2:H:14:DT:O5'	2.15	0.47
1:C:223:CYS:HB2	1:C:235:TYR:CD2	2.49	0.47
1:D:240:ILE:HD12	1:D:243:ARG:HD3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:13:DG:H4'	2:G:14:DT:O5'	2.15	0.47
1:D:87:PHE:HA	1:D:154:LEU:HD23	1.96	0.47
1:D:224:CYS:SG	1:D:235:TYR:HB3	2.55	0.47
1:A:429:MET:HE2	1:A:429:MET:HB3	1.64	0.46
1:D:76:SER:HA	1:D:79:VAL:HG22	1.97	0.46
1:D:472:ASN:ND2	1:D:472:ASN:O	2.47	0.46
1:D:490:THR:HG23	1:D:586:ILE:H	1.80	0.46
1:B:335:GLN:HG2	1:B:341:ALA:HB2	1.96	0.46
1:C:161:LEU:HB2	1:C:189:VAL:HG12	1.96	0.46
1:C:522:LYS:HG3	1:C:523:GLY:H	1.80	0.46
1:A:136:VAL:HA	1:A:217:ALA:HB3	1.98	0.46
1:D:343:ALA:HA	1:D:369:VAL:O	2.15	0.46
1:B:150:VAL:HG13	1:B:153:GLN:HE21	1.81	0.46
1:D:380:LYS:HA	1:D:381:PRO:HD3	1.66	0.46
1:A:199:MET:HE1	2:F:8:DG:H21	1.80	0.46
1:A:240:ILE:HD13	1:B:431:VAL:O	2.15	0.46
1:D:238:LEU:HD22	1:D:241:LEU:HD11	1.98	0.46
1:D:378:ILE:HG21	1:D:404:ARG:HD3	1.98	0.46
2:E:13:DG:H4'	2:E:14:DT:O5'	2.16	0.46
2:H:10:DA:H2''	2:H:11:DG:O5'	2.16	0.46
1:A:174:HIS:ND1	1:A:203:ARG:HG3	2.31	0.46
1:D:376:MET:H	1:D:378:ILE:HG13	1.81	0.46
1:A:380:LYS:HG3	1:A:383:VAL:CG2	2.46	0.46
1:B:83:LEU:HD22	1:B:92:PHE:CE2	2.51	0.46
1:C:240:ILE:HD13	1:D:432:MET:CE	2.47	0.46
1:C:328:GLU:OE1	2:G:1:DA:N6	2.49	0.46
1:C:376:MET:HE3	1:C:376:MET:HB3	1.67	0.46
1:D:352:ASP:O	1:D:356:VAL:HG23	2.16	0.45
1:D:549:PHE:HB3	1:D:555:LEU:HD13	1.98	0.45
1:A:289:GLU:HG3	1:A:476:ASP:HB3	1.98	0.45
1:C:371:THR:O	1:C:372:VAL:C	2.57	0.45
1:D:296:ASN:OD1	1:D:299:ASP:N	2.45	0.45
1:D:301:ILE:HG21	1:D:333:SER:HB2	1.97	0.45
1:C:327:SER:HB2	1:C:371:THR:HG22	1.98	0.45
1:D:554:TYR:OH	1:D:584:HIS:NE2	2.43	0.45
2:E:1:DA:H5''	2:E:1:DA:C8	2.52	0.45
1:C:359:ARG:O	1:C:364:GLU:N	2.48	0.45
1:A:240:ILE:HG21	1:B:432:MET:HE1	1.97	0.45
1:A:565:ALA:HB1	2:E:18:DT:O4	2.16	0.45
1:C:229:HIS:CD2	1:C:256:THR:HG21	2.51	0.45
1:A:182:SER:HB3	1:A:212:ARG:HH22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:VAL:HG12	1:A:254:THR:HB	1.99	0.45
1:B:436:GLY:O	1:B:440:LEU:N	2.46	0.45
1:A:96:GLN:O	1:A:100:ILE:HG12	2.16	0.45
1:A:319:ILE:HA	1:A:387:ILE:O	2.17	0.45
1:B:98:GLU:OE1	1:B:98:GLU:N	2.45	0.45
1:B:484:PHE:CD2	1:B:485:GLU:O	2.70	0.45
1:D:373:ALA:O	1:D:375:GLY:N	2.50	0.45
2:H:20:DT:H2'	2:H:20:DT:O2	2.17	0.45
1:C:136:VAL:HG22	1:C:217:ALA:HB3	1.99	0.45
1:C:242:LYS:NZ	1:C:250:LEU:HD22	2.32	0.45
1:C:319:ILE:O	1:C:369:VAL:HA	2.17	0.45
1:D:345:HIS:CE1	1:D:348:MET:HG2	2.52	0.44
1:D:376:MET:H	1:D:378:ILE:CG1	2.29	0.44
1:C:325:LYS:HE2	2:G:17:DG:OP1	2.16	0.44
1:D:308:ILE:HA	1:D:312:TYR:HD2	1.81	0.44
2:F:5:DT:H5''	2:F:5:DT:C6	2.52	0.44
1:D:490:THR:HG21	1:D:585:VAL:HA	1.98	0.44
1:D:493:CYS:O	1:D:497:ILE:HG12	2.17	0.44
1:A:392:SER:OG	1:A:401:GLU:OE1	2.32	0.44
1:A:422:ASP:HA	1:A:425:ARG:HG2	2.00	0.44
1:B:65:PRO:HB2	1:B:98:GLU:HG2	1.99	0.44
1:B:562:THR:OG1	1:B:563:ALA:N	2.51	0.44
1:C:516:ILE:O	1:C:520:MET:HG2	2.17	0.44
1:A:102:VAL:HA	1:A:107:LYS:NZ	2.32	0.44
1:A:374:PHE:O	1:A:376:MET:HG3	2.17	0.44
1:B:351:GLU:O	1:B:355:LYS:HG3	2.17	0.44
1:D:281:PHE:O	1:D:399:TYR:OH	2.25	0.44
1:D:293:LYS:HE3	1:D:422:ASP:OD2	2.17	0.44
1:D:427:SER:O	1:D:431:VAL:HG13	2.18	0.44
1:A:342:GLY:O	1:A:369:VAL:N	2.47	0.44
1:D:136:VAL:HA	1:D:217:ALA:HB3	2.00	0.44
1:D:242:LYS:HZ2	1:D:250:LEU:HD22	1.83	0.44
1:B:135:LEU:O	1:B:217:ALA:N	2.45	0.44
1:C:537:LEU:HB2	1:C:542:LEU:HD21	2.00	0.44
1:D:509:LYS:HG2	1:D:569:TYR:CD1	2.53	0.44
1:A:380:LYS:HD2	1:A:380:LYS:HA	1.52	0.43
1:D:289:GLU:HG3	1:D:476:ASP:HB3	1.99	0.43
1:C:137:ILE:HG21	1:C:238:LEU:HD11	2.00	0.43
1:C:321:CYS:N	1:C:370:ALA:O	2.30	0.43
1:D:114:PRO:HG3	1:D:281:PHE:CG	2.53	0.43
1:A:285:ASN:ND2	1:A:406:GLY:O	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ILE:HG12	1:B:434:ASN:ND2	2.34	0.43
1:A:283:ARG:NH1	1:A:403:GLY:O	2.51	0.43
1:D:307:LEU:HG	1:D:312:TYR:HE2	1.84	0.43
1:A:395:MET:HG3	1:A:461:HIS:CE1	2.54	0.43
1:A:581:ASN:ND2	1:C:452:LYS:HA	2.34	0.43
1:A:581:ASN:HD21	1:C:452:LYS:HA	1.84	0.43
1:B:436:GLY:HA2	1:B:439:LYS:HB2	2.00	0.43
1:C:510:LEU:HD22	1:C:514:LYS:HB3	2.00	0.43
1:A:166:PRO:O	1:A:170:VAL:HG23	2.19	0.43
1:B:191:PRO:HB2	1:B:234:ASP:HB3	2.01	0.43
1:B:386:VAL:CG2	1:B:405:ALA:HB2	2.48	0.43
1:D:497:ILE:HD12	1:D:572:VAL:HG22	2.01	0.43
1:A:240:ILE:HG13	1:A:244:GLN:NE2	2.34	0.43
1:A:346:ALA:HB2	2:E:20:DT:OP1	2.18	0.43
1:D:227:TRP:HB2	1:D:261:VAL:HG22	2.01	0.43
1:D:285:ASN:ND2	1:D:406:GLY:O	2.47	0.43
1:B:224:CYS:SG	1:B:269:LEU:HD11	2.59	0.42
1:C:244:GLN:OE1	1:D:561:PHE:HE1	2.02	0.42
1:A:132:GLY:HA2	1:A:212:ARG:HE	1.84	0.42
1:A:205:GLU:HG3	1:B:561:PHE:HB2	2.01	0.42
1:B:484:PHE:CE2	1:B:590:VAL:HG22	2.54	0.42
1:C:325:LYS:HA	1:C:325:LYS:HD3	1.77	0.42
1:D:482:ILE:HG21	1:D:591:LYS:HD2	2.01	0.42
1:C:113:MET:HG2	1:C:117:GLY:HA3	2.01	0.42
1:D:266:GLN:HB3	1:D:271:VAL:O	2.19	0.42
1:C:340:PRO:HB2	1:C:365:ILE:HD12	2.02	0.42
1:C:508:GLU:HG2	1:C:527:LEU:HD21	2.01	0.42
1:D:372:VAL:HG11	1:D:393:LYS:HZ2	1.85	0.42
2:G:4:DG:H4'	2:G:5:DT:H5'	2.01	0.42
1:B:456:VAL:O	1:B:460:GLN:HG3	2.20	0.42
1:A:116:GLY:H	4:A:1002:ADP:PB	2.42	0.42
1:A:269:LEU:O	1:A:271:VAL:N	2.48	0.42
1:A:328:GLU:HG3	1:A:345:HIS:NE2	2.34	0.42
1:C:498:LYS:HG3	1:C:529:VAL:HG21	2.00	0.42
1:D:312:TYR:CE1	1:D:385:PHE:HB3	2.54	0.42
1:A:282:ASN:OD1	1:A:455:ARG:HD3	2.19	0.42
1:B:260:HIS:HA	1:B:263:LYS:HG2	2.02	0.42
1:B:509:LYS:HA	1:B:509:LYS:HD3	1.80	0.42
1:B:588:MET:HE2	1:B:588:MET:HB3	1.93	0.42
1:D:225:SER:HB3	1:D:261:VAL:HG13	2.01	0.42
1:C:379:ASP:OD2	4:C:1002:ADP:O3'	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLN:HG2	1:D:90:GLN:HA	2.02	0.42
1:B:360:TRP:CD1	1:B:368:VAL:HG23	2.55	0.42
1:B:376:MET:HB2	1:B:404:ARG:HE	1.85	0.42
1:D:182:SER:HB3	1:D:212:ARG:NH1	2.30	0.42
1:D:194:ILE:HD12	1:D:241:LEU:HD21	2.02	0.42
2:E:10:DA:H2''	2:E:11:DG:H5''	2.02	0.42
1:D:62:MET:HE3	1:D:276:THR:HG22	2.02	0.42
2:G:5:DT:O2	2:G:5:DT:H2'	2.20	0.42
2:G:10:DA:H2''	2:G:11:DG:O5'	2.20	0.42
1:C:454:ARG:HG3	1:C:475:CYS:SG	2.60	0.41
1:A:340:PRO:HG2	1:A:366:GLN:H	1.85	0.41
1:A:545:ILE:HD13	1:A:588:MET:SD	2.61	0.41
1:B:488:ASN:ND2	1:B:490:THR:OG1	2.50	0.41
1:B:395:MET:HG3	1:B:461:HIS:CE1	2.55	0.41
1:C:289:GLU:HG3	1:C:476:ASP:CG	2.46	0.41
2:E:5:DT:O2	2:E:5:DT:H2'	2.20	0.41
2:H:4:DG:H4'	2:H:5:DT:H5'	2.01	0.41
1:B:266:GLN:HB3	1:B:271:VAL:O	2.19	0.41
1:C:320:TYR:CD1	1:C:372:VAL:HG12	2.56	0.41
1:C:321:CYS:O	1:C:371:THR:HA	2.21	0.41
1:C:540:GLU:O	1:C:543:GLU:HG2	2.20	0.41
2:G:9:DT:H4'	2:G:10:DA:OP1	2.18	0.41
1:C:138:CYS:SG	1:C:139:PRO:HD2	2.60	0.41
1:C:307:LEU:HG	1:C:312:TYR:HE2	1.86	0.41
1:D:401:GLU:HA	1:D:404:ARG:NH1	2.35	0.41
1:A:160:MET:C	1:A:161:LEU:HD12	2.45	0.41
1:A:432:MET:HE1	1:B:240:ILE:HG21	2.03	0.41
1:C:365:ILE:HD12	1:C:365:ILE:HA	1.90	0.41
1:C:446:TYR:CE2	1:C:454:ARG:HB3	2.56	0.41
2:E:4:DG:H2''	2:E:5:DT:OP2	2.21	0.41
2:F:10:DA:H2''	2:F:11:DG:O5'	2.20	0.41
1:A:89:LEU:HD22	4:A:1002:ADP:C2	2.55	0.41
1:B:402:SER:HB2	1:B:414:CYS:HB3	2.02	0.41
1:B:427:SER:HA	1:B:430:VAL:HG22	2.02	0.41
1:C:309:ASN:O	1:C:313:LYS:HG2	2.20	0.41
1:C:373:ALA:HB2	2:G:20:DT:C4'	2.50	0.41
1:D:484:PHE:HB3	1:D:589:ARG:HD2	2.01	0.41
1:B:283:ARG:NH2	1:B:406:GLY:O	2.54	0.41
1:B:474:MET:HB3	1:B:474:MET:HE2	1.71	0.41
1:C:386:VAL:HG23	1:C:405:ALA:HB2	2.03	0.41
1:C:430:VAL:HB	1:C:436:GLY:HA3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:LEU:HG	1:D:312:TYR:CE2	2.56	0.41
1:B:160:MET:HA	1:B:188:TYR:O	2.21	0.41
1:B:471:CYS:O	1:B:474:MET:HG2	2.21	0.41
1:B:496:LEU:HD21	1:B:519:TRP:CE3	2.56	0.41
1:D:320:TYR:HA	1:D:370:ALA:O	2.21	0.41
1:A:481:GLU:HG2	1:A:484:PHE:CE1	2.56	0.41
1:A:588:MET:HE2	1:A:588:MET:HB3	1.95	0.41
1:B:227:TRP:HB2	1:B:261:VAL:HG22	2.02	0.41
1:B:344:TYR:HD1	1:B:356:VAL:HG21	1.87	0.40
1:D:387:ILE:HG13	1:D:415:ILE:HB	2.02	0.40
1:D:446:TYR:CE1	1:D:454:ARG:HD2	2.56	0.40
1:A:146:ASP:HA	1:A:149:MET:HE3	2.02	0.40
1:A:273:LYS:HD2	1:A:273:LYS:HA	1.91	0.40
1:B:485:GLU:OE1	1:B:592:LYS:HE2	2.20	0.40
1:C:344:TYR:CE1	1:C:353:LYS:HB3	2.55	0.40
1:C:378:ILE:O	1:C:378:ILE:HG22	2.21	0.40
1:C:532:LEU:HD23	1:C:532:LEU:HA	1.85	0.40
1:C:224:CYS:SG	1:C:235:TYR:HB3	2.62	0.40
1:A:93:ARG:HB3	1:A:94:PRO:HD2	2.04	0.40
1:A:170:VAL:HG12	1:A:174:HIS:CD2	2.56	0.40
1:A:225:SER:HB3	1:A:261:VAL:HG13	2.04	0.40
1:C:224:CYS:HA	1:C:235:TYR:HB3	2.03	0.40
2:F:5:DT:O2	2:F:5:DT:H2'	2.20	0.40
2:E:4:DG:H4'	2:E:5:DT:H5'	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	529/531 (100%)	529 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	529/531 (100%)	529 (100%)	0	0	100	100
1	C	529/531 (100%)	529 (100%)	0	0	100	100
1	D	529/531 (100%)	525 (99%)	4 (1%)	0	100	100
All	All	2116/2124 (100%)	2112 (100%)	4 (0%)	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	469/469 (100%)	460 (98%)	9 (2%)	52	76
1	B	469/469 (100%)	457 (97%)	12 (3%)	41	70
1	C	469/469 (100%)	461 (98%)	8 (2%)	56	78
1	D	469/469 (100%)	458 (98%)	11 (2%)	45	72
All	All	1876/1876 (100%)	1836 (98%)	40 (2%)	48	74

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	301	ILE
1	A	305	VAL
1	A	347	ASN
1	A	356	VAL
1	A	374	PHE
1	A	378	ILE
1	A	423	ILE
1	A	456	VAL
1	A	566	THR
1	B	150	VAL
1	B	156	ILE
1	B	170	VAL
1	B	214	THR

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Mol	Chain	Res	Type
1	B	258	THR
1	B	345	HIS
1	B	367	VAL
1	B	369	VAL
1	B	376	MET
1	B	378	ILE
1	B	387	ILE
1	B	474	MET
1	C	345	HIS
1	C	351	GLU
1	C	354	THR
1	C	367	VAL
1	C	371	THR
1	C	374	PHE
1	C	456	VAL
1	C	585	VAL
1	D	86	VAL
1	D	242	LYS
1	D	308	ILE
1	D	345	HIS
1	D	347	ASN
1	D	376	MET
1	D	378	ILE
1	D	386	VAL
1	D	489	VAL
1	D	529	VAL
1	D	572	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	179	ASN
1	A	389	HIS
1	A	449	ASN
1	A	580	ASN
1	B	153	GLN
1	B	347	ASN
1	B	580	ASN
1	C	315	GLN
1	C	347	ASN
1	C	357	HIS
1	C	548	HIS

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Mol	Chain	Res	Type
1	D	229	HIS
1	D	324	GLN
1	D	335	GLN
1	D	388	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 19 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	ADP	B	1002	5	22,28,29	0.97	1 (4%)	23,42,45	1.34	3 (13%)
6	PO4	B	1004	-	4,4,4	1.49	1 (25%)	6,6,6	0.47	0
4	ADP	C	1002	5	22,28,29	0.99	1 (4%)	23,42,45	1.52	5 (21%)
4	ADP	D	1002	5	24,29,29	0.94	1 (4%)	29,45,45	1.36	4 (13%)
4	ADP	A	1002	5	22,28,29	0.99	1 (4%)	23,42,45	1.36	2 (8%)
6	PO4	F	104	-	4,4,4	1.51	1 (25%)	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	C	1002	5	-	5/9/31/32	0/3/3/3
4	ADP	B	1002	5	-	5/9/31/32	0/3/3/3
4	ADP	D	1002	5	-	6/12/32/32	0/3/3/3
4	ADP	A	1002	5	-	5/9/31/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	104	PO4	P-O1	2.60	1.57	1.50
6	B	1004	PO4	P-O1	2.58	1.56	1.50
4	B	1002	ADP	C5-C4	2.47	1.47	1.40
4	D	1002	ADP	C5-C4	2.46	1.47	1.40
4	A	1002	ADP	C5-C4	2.42	1.47	1.40
4	C	1002	ADP	C5-C4	2.29	1.47	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1002	ADP	N3-C2-N1	-3.43	123.31	128.68
4	D	1002	ADP	N3-C2-N1	-3.19	123.69	128.68
4	A	1002	ADP	N3-C2-N1	-3.18	123.71	128.68
4	B	1002	ADP	N3-C2-N1	-3.18	123.71	128.68
4	C	1002	ADP	C4-C5-N7	-2.76	106.53	109.40
4	A	1002	ADP	C4-C5-N7	-2.61	106.68	109.40
4	B	1002	ADP	C3'-C2'-C1'	2.58	104.87	100.98
4	B	1002	ADP	C4-C5-N7	-2.54	106.75	109.40
4	C	1002	ADP	C1'-N9-C4	-2.53	122.19	126.64
4	D	1002	ADP	PA-O3A-PB	-2.49	124.27	132.83
4	D	1002	ADP	C3'-C2'-C1'	2.46	104.69	100.98
4	D	1002	ADP	C4-C5-N7	-2.45	106.85	109.40
4	C	1002	ADP	O3'-C3'-C2'	-2.20	104.71	111.82
4	C	1002	ADP	C2'-C3'-C4'	2.10	106.72	102.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	ADP	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
4	B	1002	ADP	C5'-O5'-PA-O2A
4	C	1002	ADP	C5'-O5'-PA-O2A
4	D	1002	ADP	PA-O3A-PB-O2B
4	D	1002	ADP	PA-O3A-PB-O3B
4	D	1002	ADP	C5'-O5'-PA-O2A
4	B	1002	ADP	O4'-C4'-C5'-O5'
4	A	1002	ADP	C5'-O5'-PA-O3A
4	B	1002	ADP	C5'-O5'-PA-O3A
4	C	1002	ADP	C5'-O5'-PA-O3A
4	D	1002	ADP	C5'-O5'-PA-O3A
4	A	1002	ADP	C5'-O5'-PA-O1A
4	B	1002	ADP	C5'-O5'-PA-O1A
4	C	1002	ADP	C5'-O5'-PA-O1A
4	D	1002	ADP	C5'-O5'-PA-O1A
4	B	1002	ADP	C3'-C4'-C5'-O5'
4	A	1002	ADP	C3'-C4'-C5'-O5'
4	A	1002	ADP	O4'-C4'-C5'-O5'
4	C	1002	ADP	O4'-C4'-C5'-O5'
4	D	1002	ADP	O4'-C4'-C5'-O5'
4	C	1002	ADP	C3'-C4'-C5'-O5'

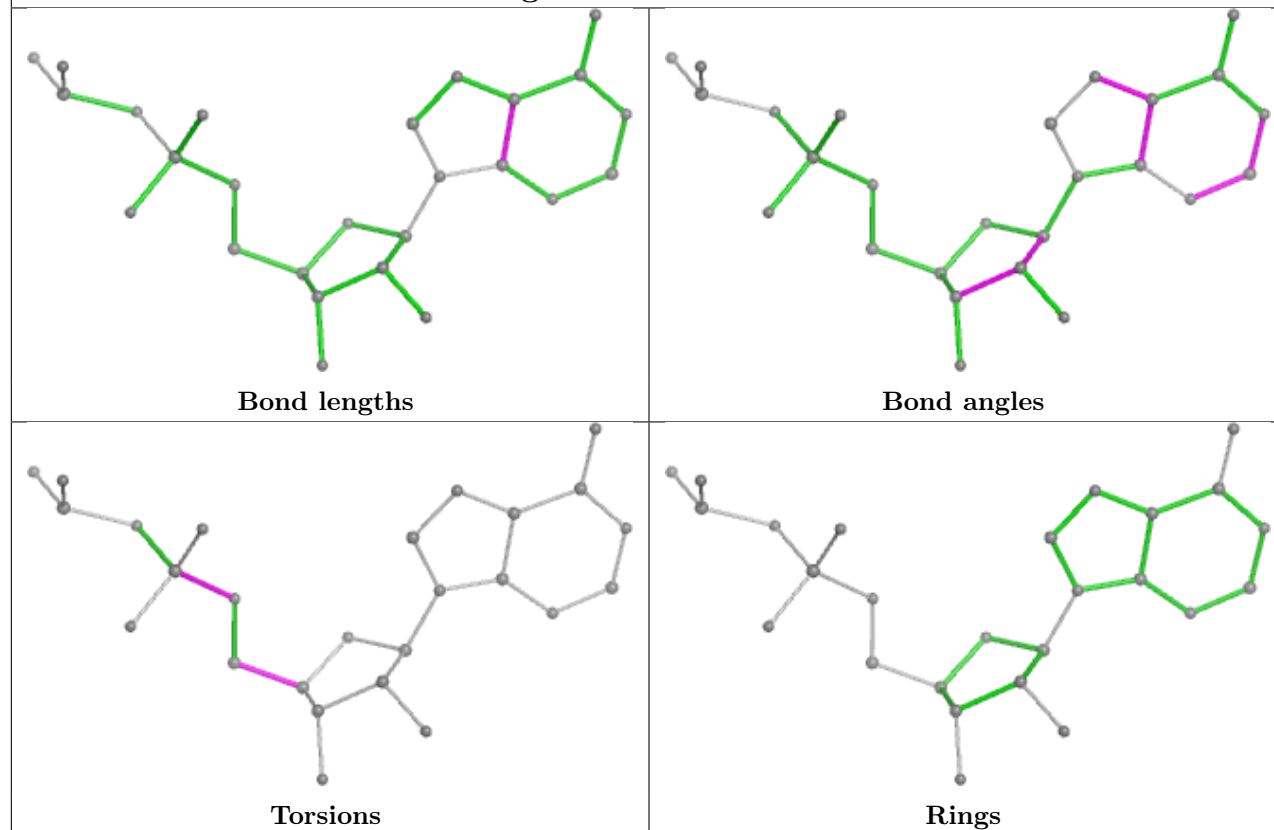
There are no ring outliers.

4 monomers are involved in 9 short contacts:

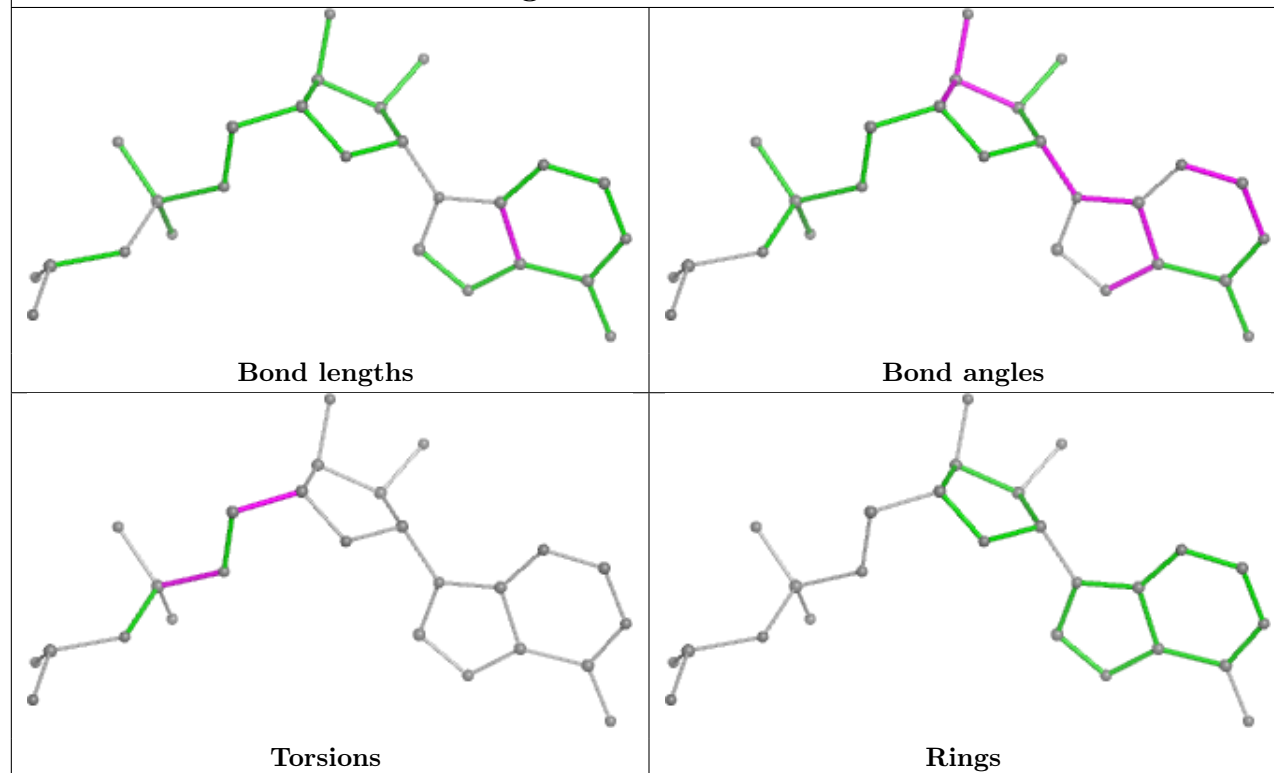
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1004	PO4	1	0
4	C	1002	ADP	2	0
4	D	1002	ADP	1	0
4	A	1002	ADP	5	0

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.

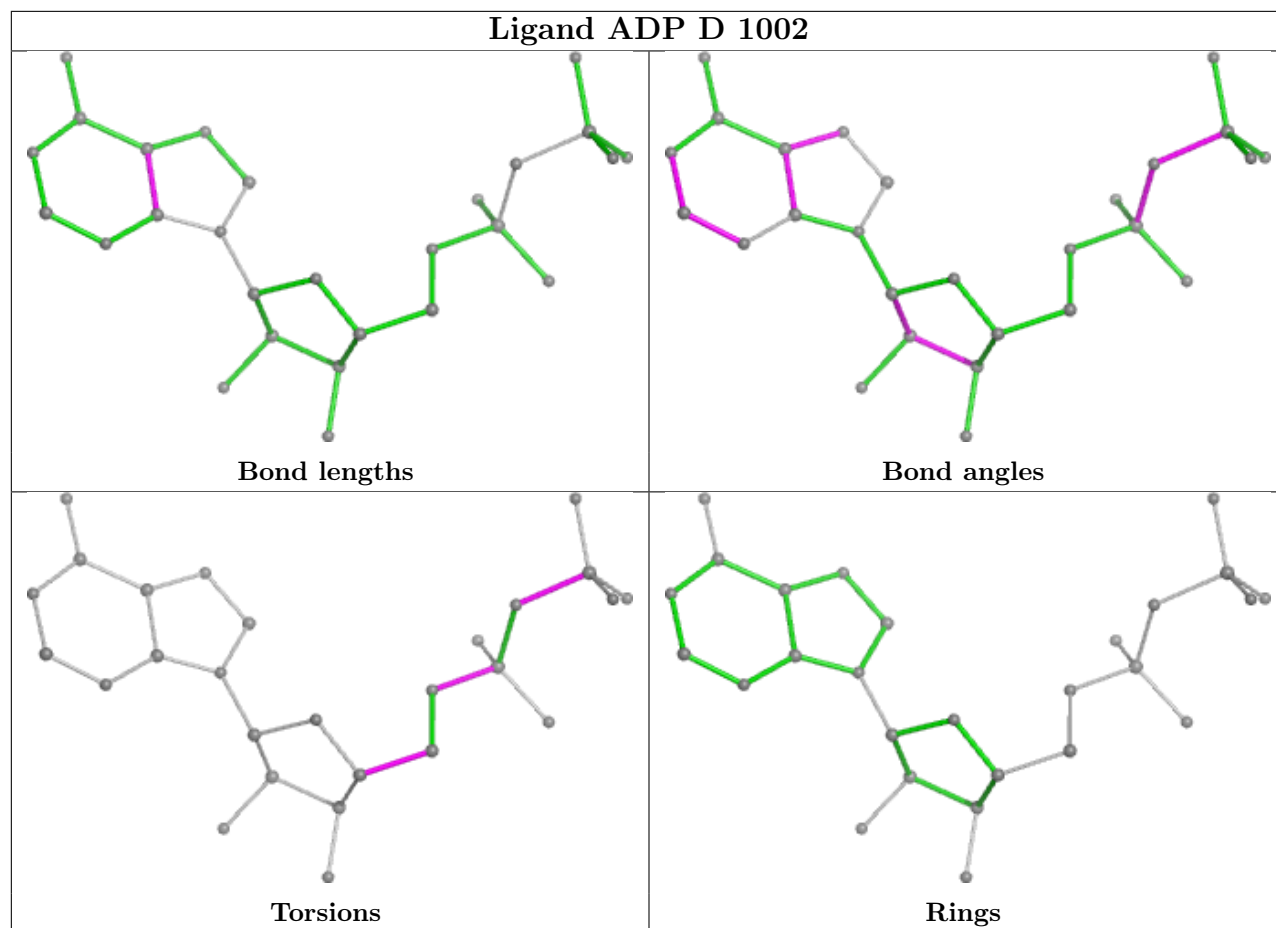
Ligand ADP B 1002



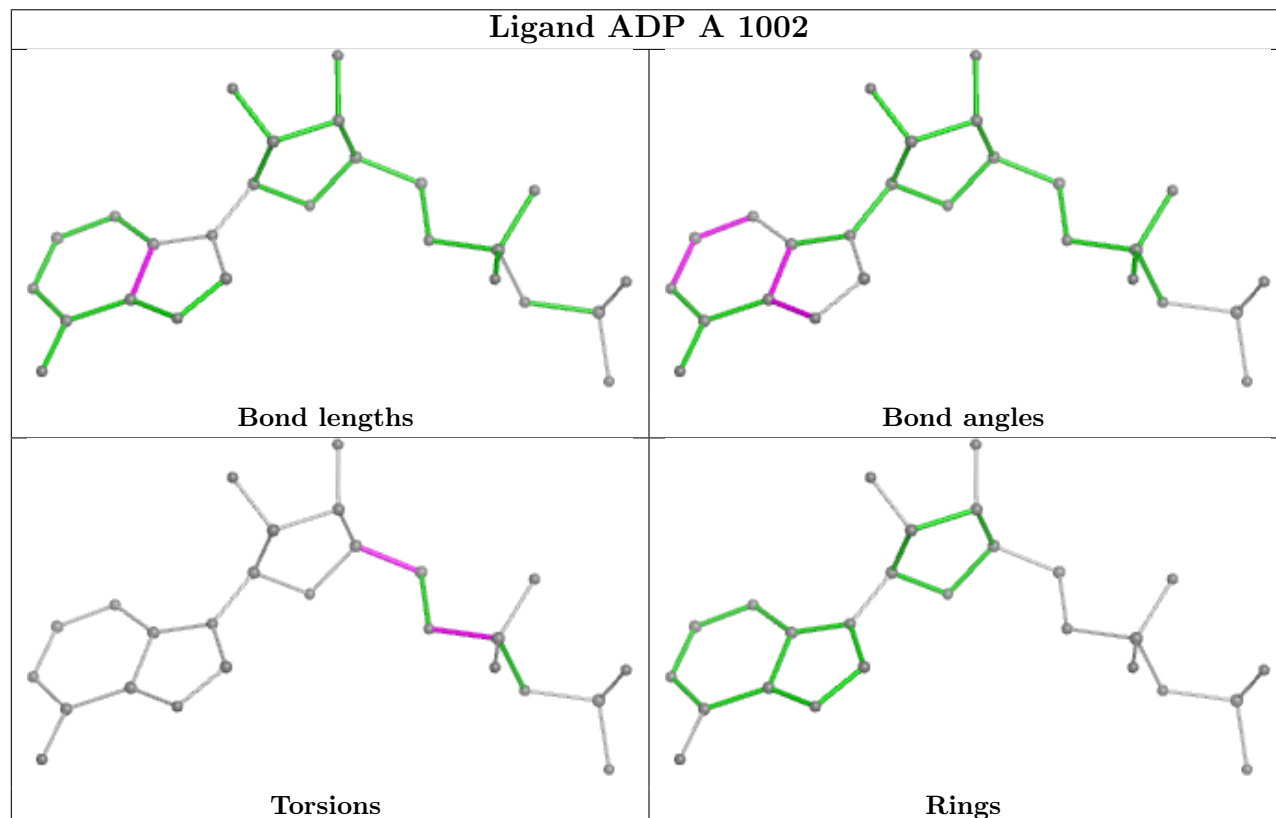
Ligand ADP C 1002



Ligand ADP D 1002



Ligand ADP A 1002



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	531/531 (100%)	-0.13	3 (0%) 85 76	66, 99, 151, 257	0
1	B	531/531 (100%)	-0.14	3 (0%) 85 76	53, 95, 144, 208	0
1	C	531/531 (100%)	-0.07	9 (1%) 69 53	67, 96, 137, 214	0
1	D	531/531 (100%)	-0.08	6 (1%) 77 63	65, 98, 134, 217	0
2	E	21/24 (87%)	0.24	0 100 100	103, 108, 174, 198	0
2	F	19/24 (79%)	0.07	1 (5%) 33 22	102, 117, 211, 228	0
2	G	21/24 (87%)	0.31	1 (4%) 36 25	96, 118, 169, 193	0
2	H	21/24 (87%)	0.08	1 (4%) 36 25	97, 110, 156, 196	0
All	All	2206/2220 (99%)	-0.10	24 (1%) 77 63	53, 98, 146, 257	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	567	ILE	3.8
1	D	341	ALA	3.7
1	D	563	ALA	3.3
1	C	341	ALA	3.3
1	B	213	PHE	3.3
1	A	376	MET	3.2
1	C	213	PHE	3.1
1	C	319	ILE	3.1
1	C	569	TYR	3.0
1	C	205	GLU	2.6
2	G	21	DT	2.6
1	B	357	HIS	2.6
1	C	386	VAL	2.6
1	D	312	TYR	2.5
1	B	563	ALA	2.5
2	F	20	DT	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	290	VAL	2.3
2	H	21	DT	2.3
1	D	564	TYR	2.3
1	C	378	ILE	2.2
1	C	385	PHE	2.1
1	A	341	ALA	2.1
1	A	256	THR	2.0
1	D	567	ILE	2.0

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

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

6.3 Carbohydrates ⓘ

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(\AA^2)	Q<0.9
5	MG	D	1003	1/1	0.51	0.38	82,82,82,82	0
6	PO4	B	1004	5/5	0.57	0.10	131,135,167,308	0
5	MG	B	1003	1/1	0.69	0.27	66,66,66,66	0
6	PO4	F	104	5/5	0.70	0.10	128,133,136,136	5
5	MG	A	1003	1/1	0.76	0.23	66,66,66,66	0
4	ADP	D	1002	27/27	0.83	0.11	75,101,118,126	0
5	MG	C	1003	1/1	0.84	0.24	65,65,65,65	0
4	ADP	B	1002	26/27	0.85	0.11	57,82,99,109	0
4	ADP	C	1002	26/27	0.86	0.11	67,95,110,121	0
4	ADP	A	1002	26/27	0.88	0.09	77,108,128,143	0
7	K	E	102	1/1	0.93	0.05	87,87,87,87	0
7	K	E	103	1/1	0.96	0.07	102,102,102,102	1
7	K	F	103	1/1	0.96	0.06	95,95,95,95	1
7	K	G	102	1/1	0.96	0.07	89,89,89,89	0
7	K	E	101	1/1	0.97	0.06	79,79,79,79	0

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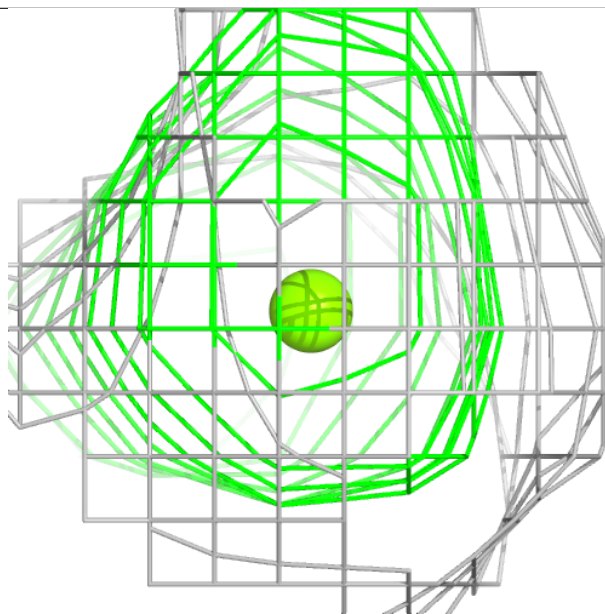
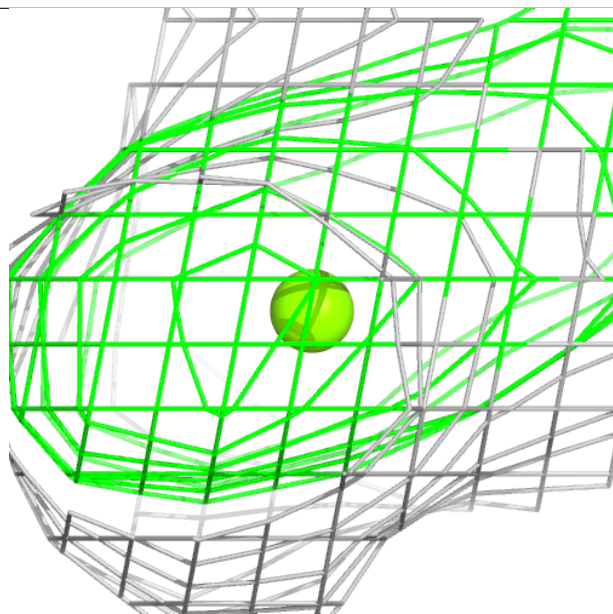
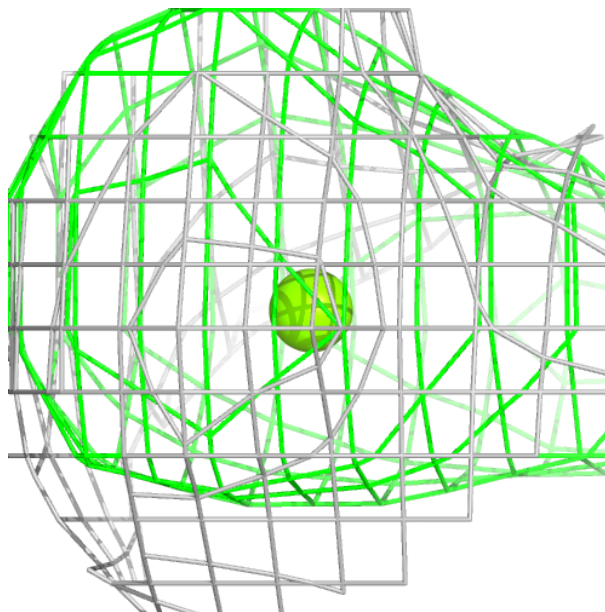
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	K	F	101	1/1	0.97	0.03	75,75,75,75	0
7	K	H	101	1/1	0.97	0.05	83,83,83,83	1
7	K	G	101	1/1	0.98	0.07	88,88,88,88	0
7	K	F	102	1/1	0.98	0.03	91,91,91,91	0
3	ZN	C	1001	1/1	0.98	0.03	73,73,73,73	0
7	K	H	102	1/1	0.98	0.04	94,94,94,94	0
7	K	H	103	1/1	0.98	0.06	95,95,95,95	0
3	ZN	B	1001	1/1	0.99	0.03	83,83,83,83	0
3	ZN	A	1001	1/1	0.99	0.06	131,131,131,131	0
3	ZN	D	1001	1/1	0.99	0.04	103,103,103,103	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.

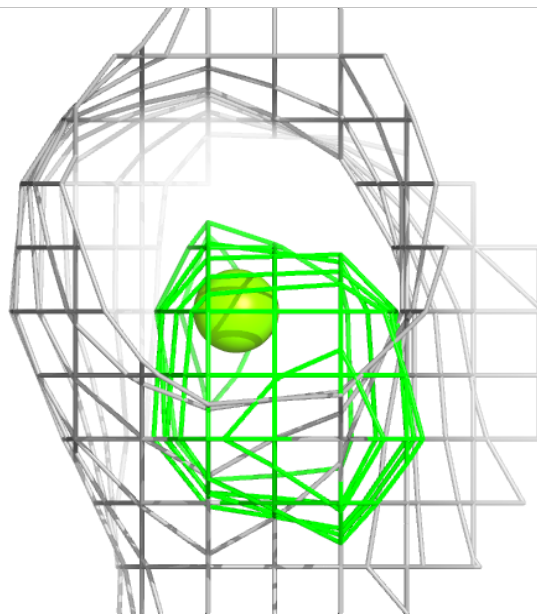
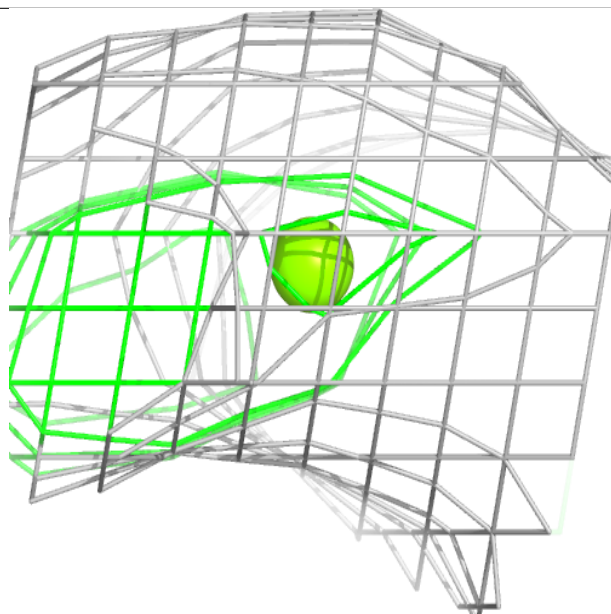
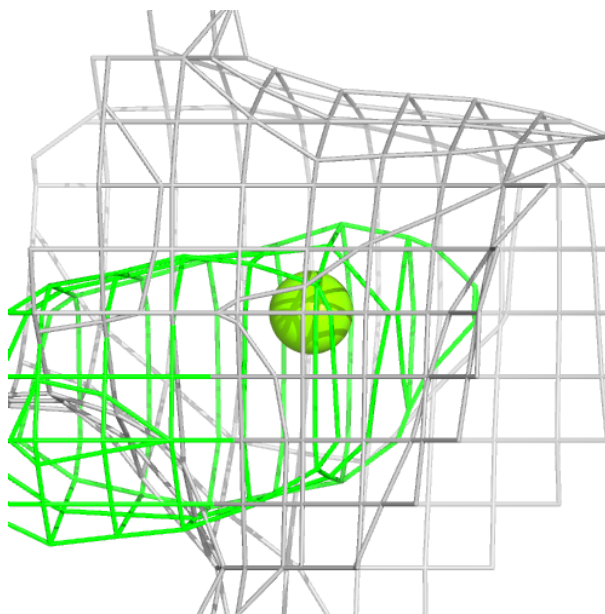
Electron density around MG D 1003:

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



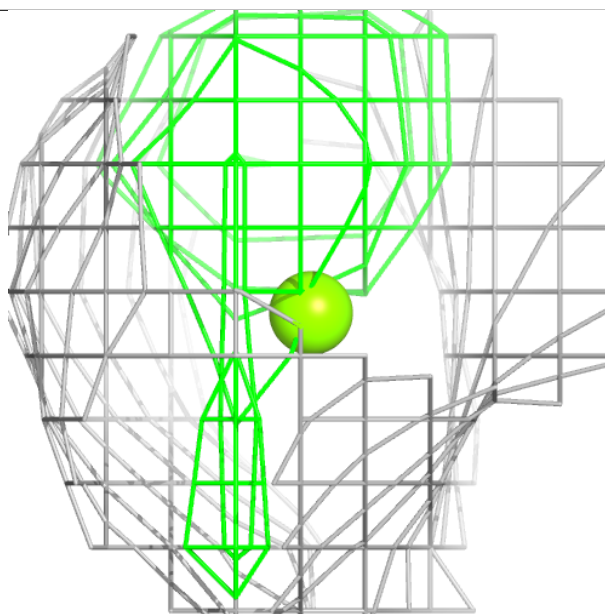
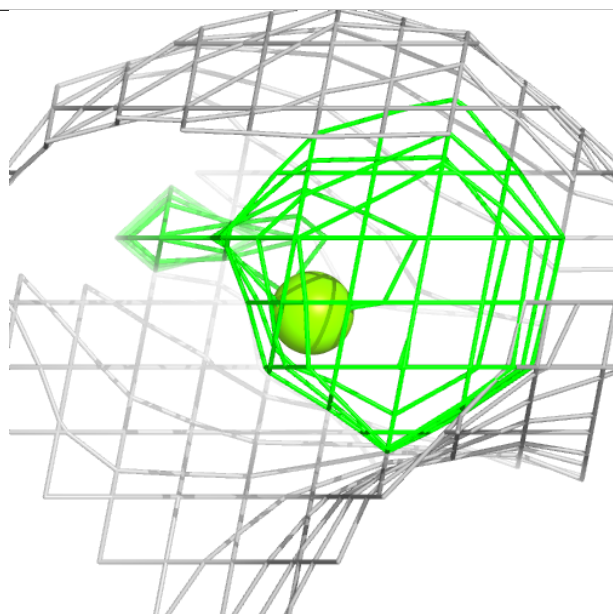
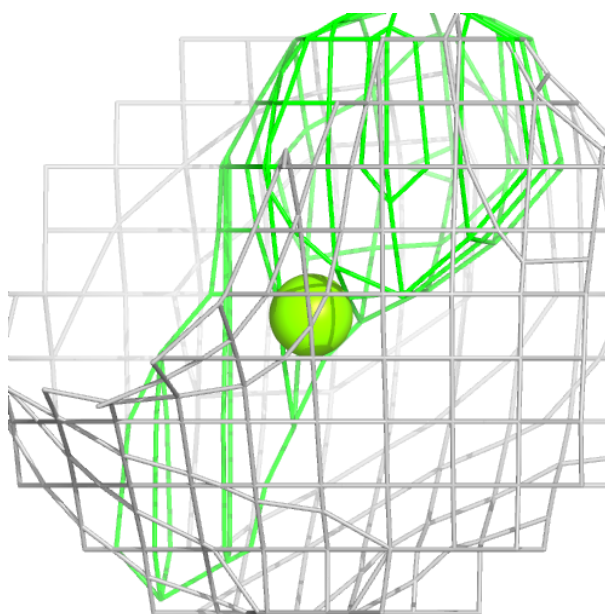
Electron density around MG B 1003:

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



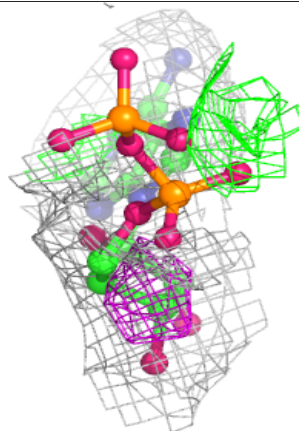
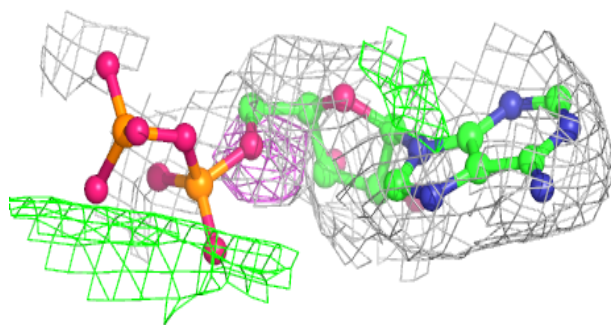
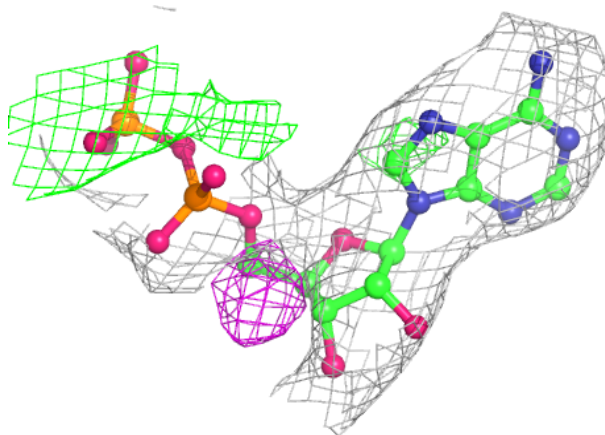
Electron density around MG A 1003:

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and green (positive)



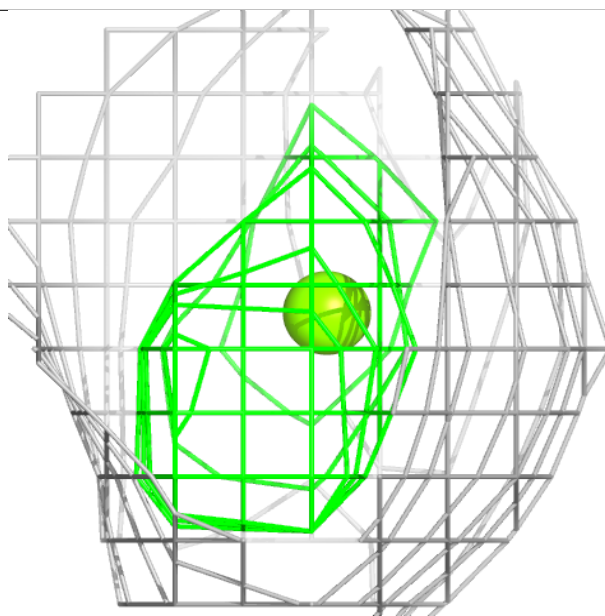
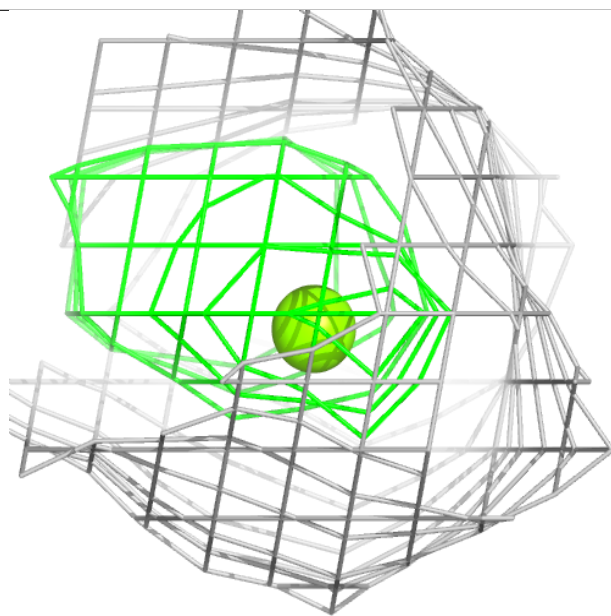
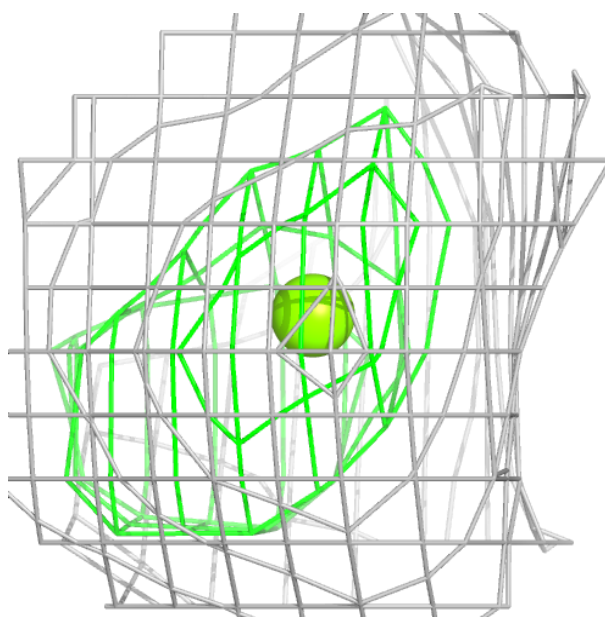
Electron density around ADP D 1002:

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and green (positive)



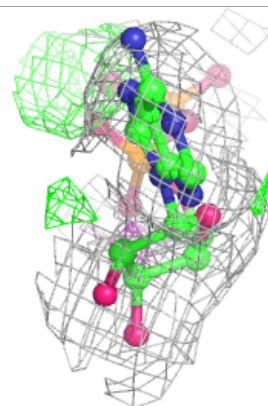
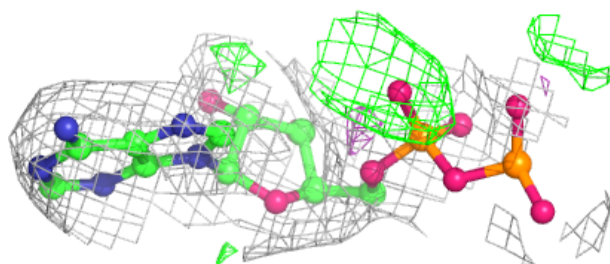
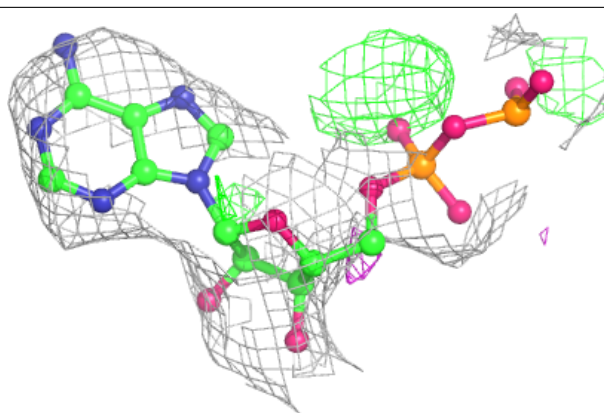
Electron density around MG C 1003:

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and green (positive)

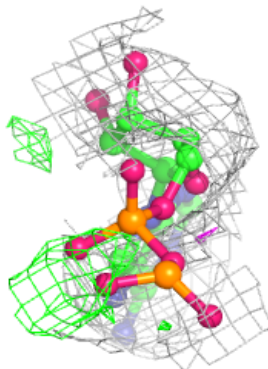
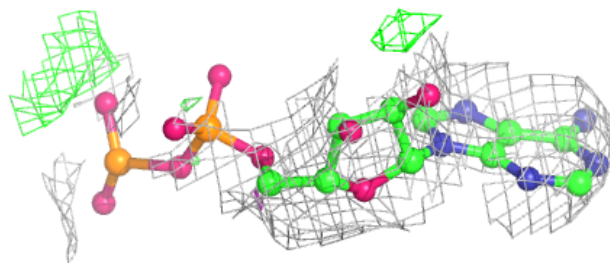
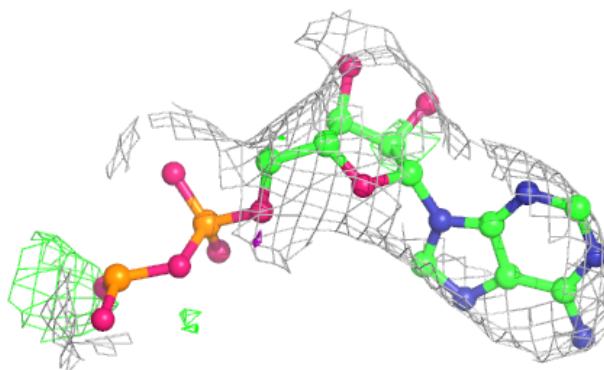


Electron density around ADP B 1002:

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

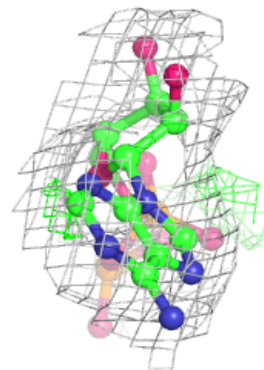
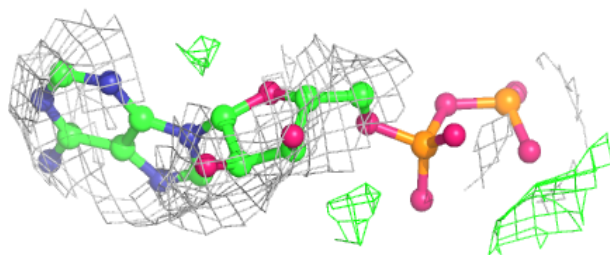
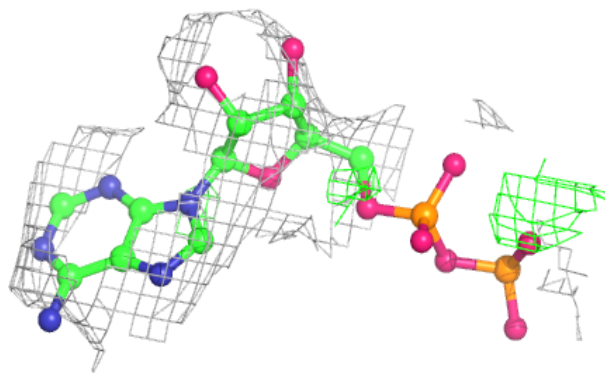
**Electron density around ADP C 1002:**

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



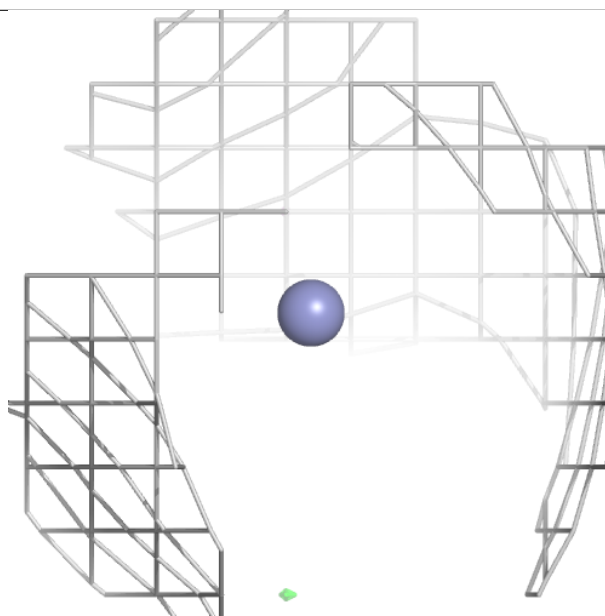
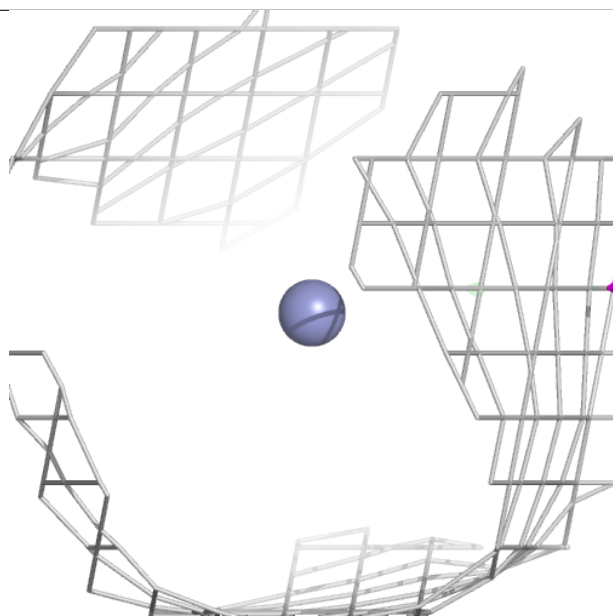
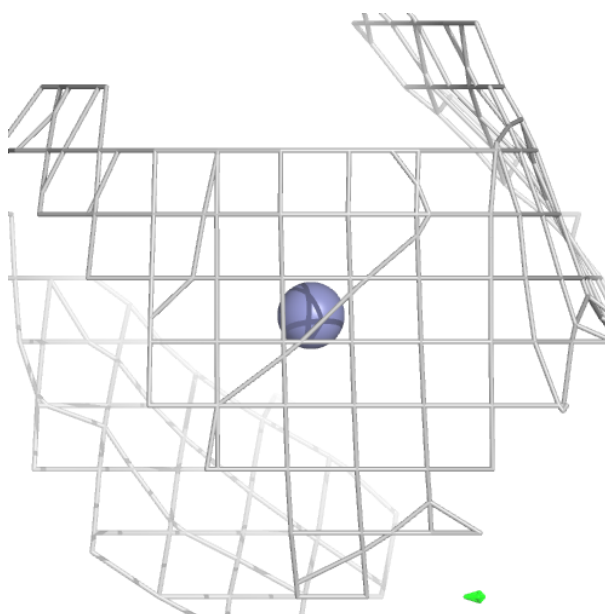
Electron density around ADP A 1002:

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and green (positive)



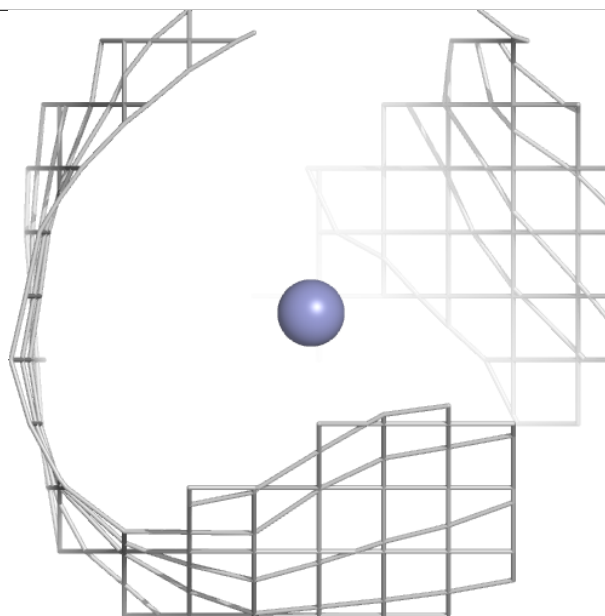
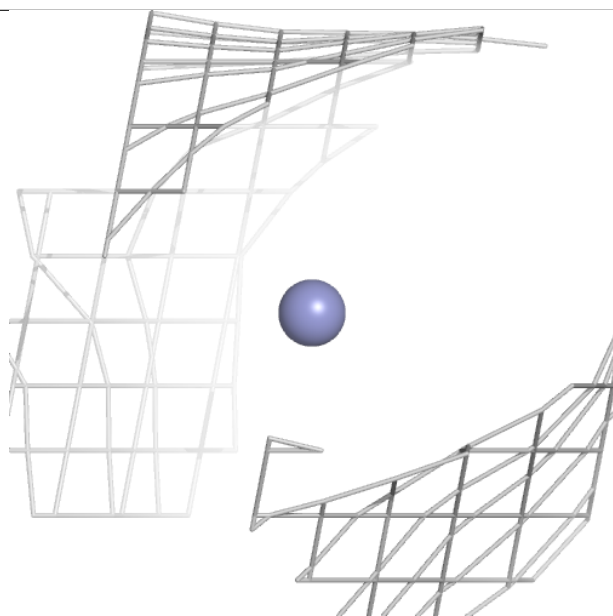
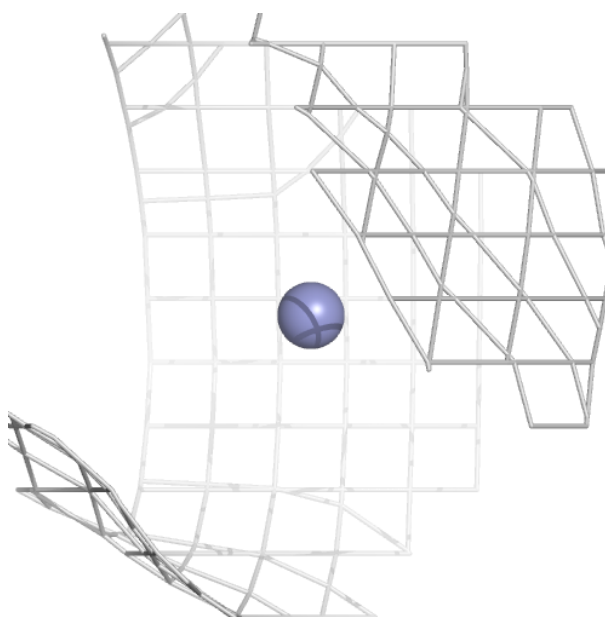
Electron density around ZN C 1001:

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



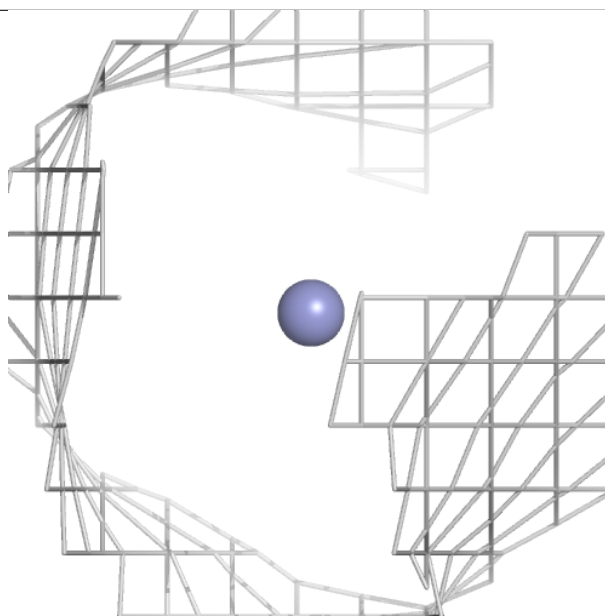
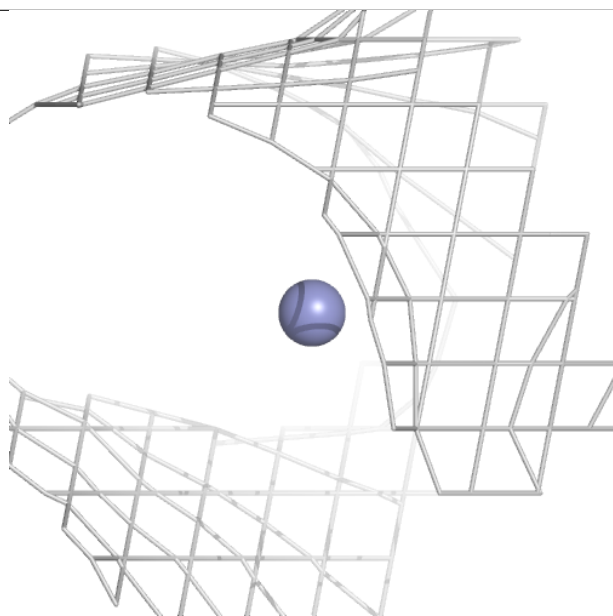
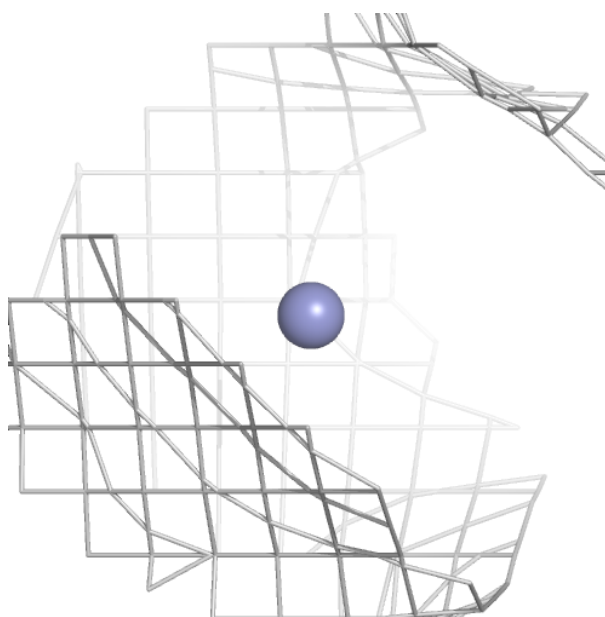
Electron density around ZN B 1001:

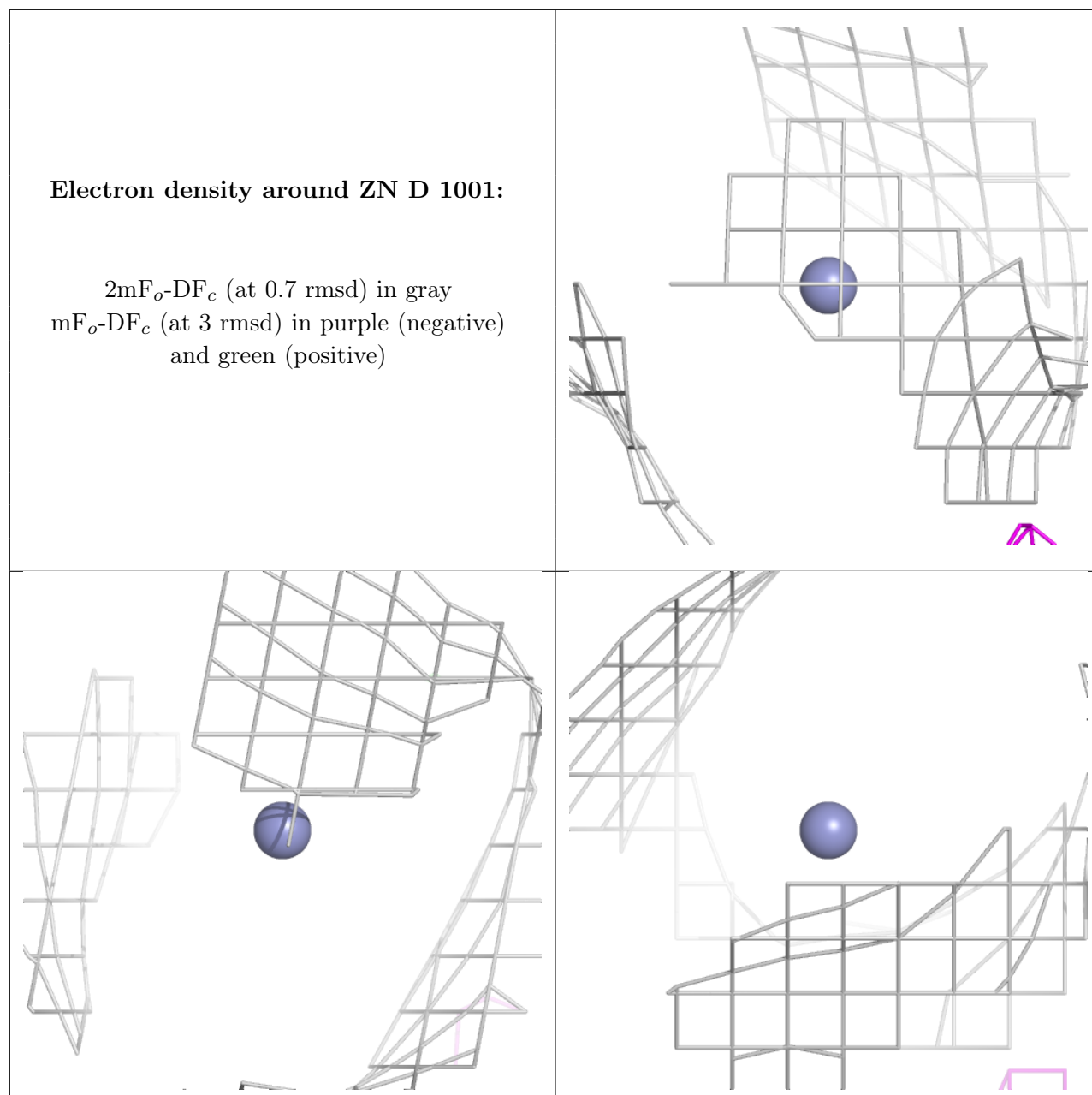
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.