



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 10:56 AM EDT

PDB ID : 8A3V / pdb_00008a3v
Title : Crystal structure of the Vibrio cholerae replicative helicase (VcDnaB) in complex with its loader protein (VcDciA)
Authors : Walbott, H.; Quevillon-Cheruel, S.; Cargemel, C.
Deposited on : 2022-06-09
Resolution : 2.90 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

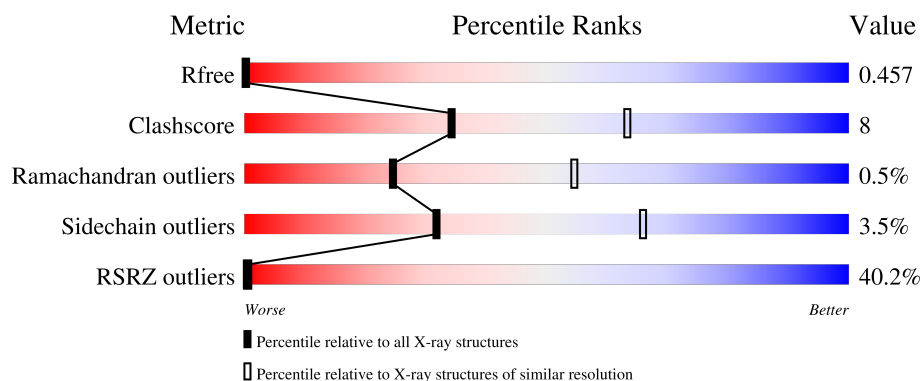
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	474	
1	B	474	
2	C	163	
2	D	163	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9367 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 Replicative DNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3509	2184	619	691	15			
1	B	447	Total	C	N	O	S	0	0	0
			3481	2168	611	687	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	469	HIS	-	expression tag	UNP A0A085R2T8
A	470	HIS	-	expression tag	UNP A0A085R2T8
A	471	HIS	-	expression tag	UNP A0A085R2T8
A	472	HIS	-	expression tag	UNP A0A085R2T8
A	473	HIS	-	expression tag	UNP A0A085R2T8
A	474	HIS	-	expression tag	UNP A0A085R2T8
B	469	HIS	-	expression tag	UNP A0A085R2T8
B	470	HIS	-	expression tag	UNP A0A085R2T8
B	471	HIS	-	expression tag	UNP A0A085R2T8
B	472	HIS	-	expression tag	UNP A0A085R2T8
B	473	HIS	-	expression tag	UNP A0A085R2T8
B	474	HIS	-	expression tag	UNP A0A085R2T8

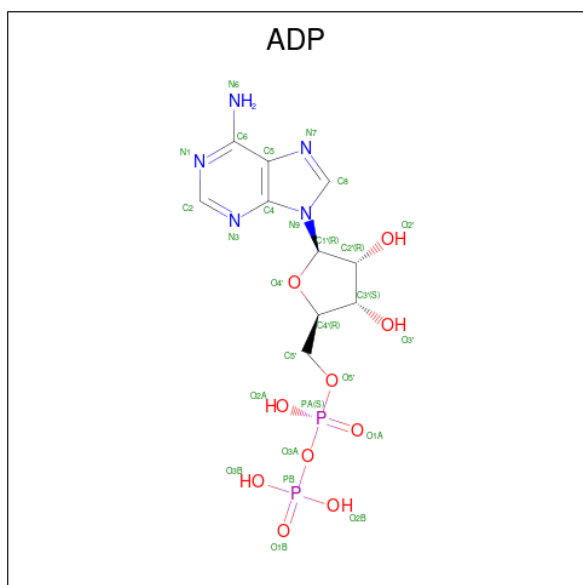
- Molecule 2 is a protein called DUF721 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	149	Total	C	N	O	S	0	0	0
			1162	726	224	211	1			
2	D	148	Total	C	N	O	S	0	0	0
			1159	723	223	212	1			

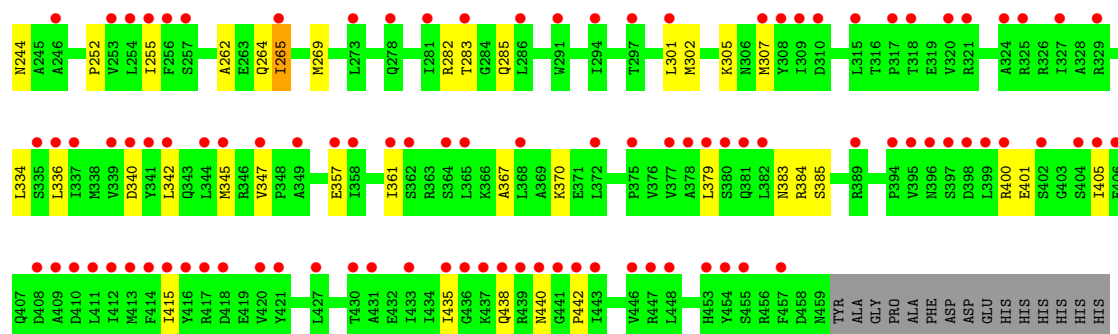
There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	initiating methionine	UNP A0A0H5ZA06
C	-4	HIS	-	expression tag	UNP A0A0H5ZA06
C	-3	HIS	-	expression tag	UNP A0A0H5ZA06
C	-2	HIS	-	expression tag	UNP A0A0H5ZA06
C	-1	HIS	-	expression tag	UNP A0A0H5ZA06
C	0	HIS	-	expression tag	UNP A0A0H5ZA06
C	1	HIS	-	expression tag	UNP A0A0H5ZA06
D	-5	MET	-	initiating methionine	UNP A0A0H5ZA06
D	-4	HIS	-	expression tag	UNP A0A0H5ZA06
D	-3	HIS	-	expression tag	UNP A0A0H5ZA06
D	-2	HIS	-	expression tag	UNP A0A0H5ZA06
D	-1	HIS	-	expression tag	UNP A0A0H5ZA06
D	0	HIS	-	expression tag	UNP A0A0H5ZA06
D	1	HIS	-	expression tag	UNP A0A0H5ZA06

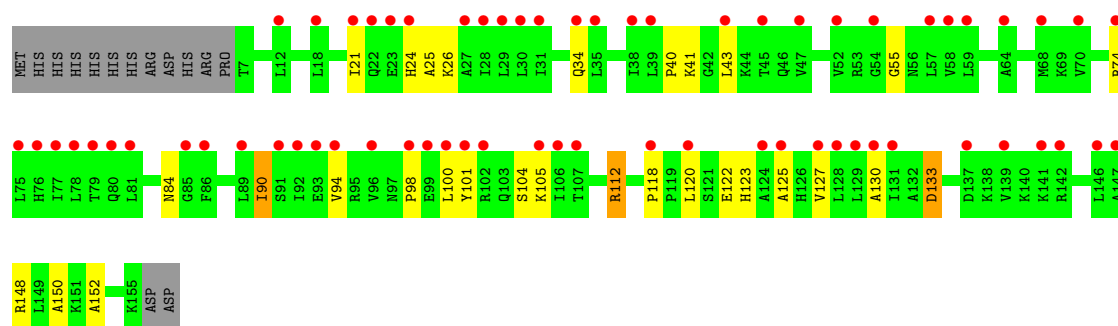
- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



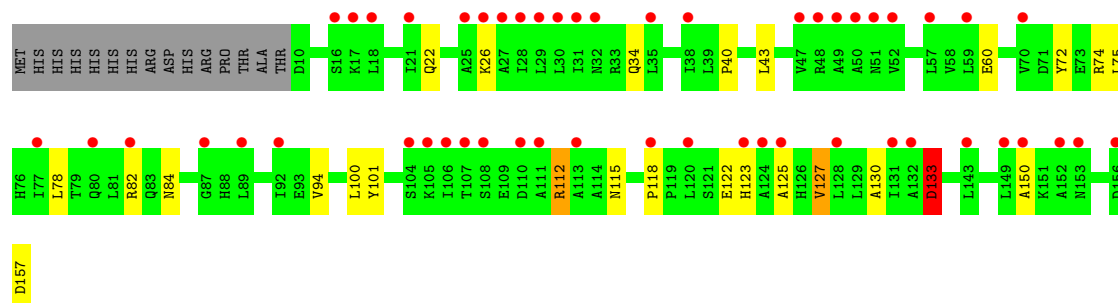
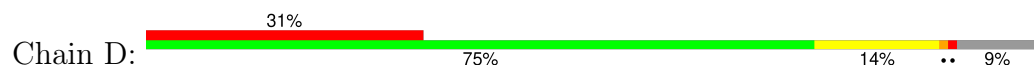
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0



● Molecule 2: DUF721 domain-containing protein



● Molecule 2: DUF721 domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	186.51Å 186.51Å 252.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.80 – 2.90 40.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	54.0 (40.80-2.90) 54.0 (40.80-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3 (20-MAY-2020)	Depositor
R, R_{free}	0.279 , 0.290 0.429 , 0.457	Depositor DCC
R_{free} test set	1229 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	84.7	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 103.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9367	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: MG, ADP

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	0.52	1/3558 (0.0%)	0.93	3/4811 (0.1%)
1	B	0.51	0/3530	0.94	3/4775 (0.1%)
2	C	0.55	0/1174	1.05	3/1581 (0.2%)
2	D	0.54	0/1171	1.02	2/1576 (0.1%)
All	All	0.52	1/9433 (0.0%)	0.96	11/12743 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	ILE	CG1-CD1	-6.04	1.28	1.51

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	118	PRO	N-CA-C	7.45	119.79	110.70
2	D	118	PRO	N-CA-C	7.24	119.53	110.70
1	A	41	ASP	CA-C-N	6.55	129.94	120.38
1	A	41	ASP	C-N-CA	6.55	129.94	120.38
1	B	167	GLU	CB-CG-CD	6.19	123.12	112.60
1	B	41	ASP	CA-C-N	6.09	133.18	121.54
1	B	41	ASP	C-N-CA	6.09	133.18	121.54
2	C	152	ALA	CA-C-N	5.98	130.62	122.07
2	C	152	ALA	C-N-CA	5.98	130.62	122.07
1	A	80	ASP	CA-CB-CG	5.64	118.24	112.60
2	D	133	ASP	CA-CB-CG	5.31	117.91	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3509	0	3522	59	0
1	B	3481	0	3490	56	0
2	C	1162	0	1235	21	0
2	D	1159	0	1224	24	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9367	0	9495	144	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 8.

All (144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASP:O	1:A:379:LEU:HB2	1.65	0.96
1:B:28:LEU:HD13	1:B:62:HIS:HE1	1.32	0.94
1:B:340:ASP:O	1:B:379:LEU:HB2	1.65	0.94
1:B:264:GLN:HG3	1:B:282:ARG:HH22	1.33	0.93
1:A:264:GLN:HG3	1:A:282:ARG:HH22	1.33	0.92
2:D:22:GLN:HE21	2:D:26:LYS:NZ	1.72	0.87
2:C:21:ILE:HA	2:C:25:ALA:HB3	1.62	0.82
2:C:34:GLN:HE22	2:C:84:ASN:ND2	1.80	0.80
1:A:151:ALA:CB	1:B:125:GLU:HG3	2.12	0.80
1:B:28:LEU:HD13	1:B:62:HIS:CE1	2.17	0.78
2:D:22:GLN:HE21	2:D:26:LYS:HZ3	1.31	0.76
1:A:435:ILE:CG1	1:A:443:ILE:HA	2.15	0.76
1:A:435:ILE:HG13	1:A:443:ILE:HA	1.67	0.75
1:A:296:SER:HA	2:D:75:LEU:HD13	1.69	0.75
1:A:151:ALA:HB2	1:B:125:GLU:HG3	1.72	0.71
2:C:101:TYR:HB3	2:C:104:SER:HB3	1.75	0.69
1:A:163:PHE:HE1	1:A:325:ARG:NH1	1.93	0.67
1:B:302:MET:O	1:B:305:LYS:HG3	1.96	0.66
1:A:435:ILE:HD11	1:A:438:GLN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HB3	1:B:125:GLU:HG3	1.77	0.65
1:A:302:MET:O	1:A:305:LYS:HG3	1.97	0.65
1:B:262:ALA:O	1:B:265:ILE:HG13	1.98	0.64
1:A:383:ASN:HD22	1:A:385:SER:H	1.45	0.63
2:D:22:GLN:NE2	2:D:26:LYS:HZ3	1.97	0.63
1:B:238:ALA:HB2	1:B:379:LEU:HD21	1.80	0.63
2:C:55:GLY:HA3	2:C:90:ILE:HD13	1.79	0.62
1:A:238:ALA:HB2	1:A:379:LEU:HD21	1.81	0.62
2:C:100:LEU:HB3	2:C:105:LYS:NZ	2.15	0.62
1:B:383:ASN:HD22	1:B:385:SER:H	1.46	0.62
1:B:59:SER:OG	1:B:61:PRO:HD2	2.00	0.61
1:A:282:ARG:NH2	1:B:440:ASN:OD1	2.34	0.60
2:D:22:GLN:HG2	2:D:26:LYS:HZ3	1.66	0.60
1:B:14:PRO:HA	1:B:17:GLN:HG2	1.84	0.59
1:A:59:SER:OG	1:A:61:PRO:HD2	2.02	0.59
1:A:435:ILE:CD1	1:A:438:GLN:HB2	2.34	0.58
1:A:435:ILE:HG12	1:A:443:ILE:HA	1.84	0.57
1:B:135:VAL:HG21	1:B:165:ILE:HD11	1.86	0.57
1:A:14:PRO:HA	1:A:17:GLN:HG2	1.84	0.57
1:A:283:THR:OG1	1:A:285:GLN:HG2	2.05	0.57
2:D:60:GLU:CB	2:D:100:LEU:HD11	2.35	0.56
1:B:283:THR:OG1	1:B:285:GLN:HG2	2.05	0.56
2:C:123:HIS:ND1	2:D:72:TYR:CZ	2.74	0.56
1:A:163:PHE:HE1	1:A:325:ARG:HH11	1.54	0.55
1:A:135:VAL:HG21	1:A:165:ILE:HD11	1.88	0.55
1:B:45:TRP:HB2	1:B:73:LEU:HD13	1.89	0.55
1:A:45:TRP:HB2	1:A:73:LEU:HD13	1.89	0.55
2:C:21:ILE:CG2	2:C:26:LYS:HG3	2.36	0.55
2:D:22:GLN:CG	2:D:26:LYS:HZ3	2.20	0.55
1:A:151:ALA:HB2	1:B:125:GLU:CG	2.35	0.55
1:A:225:ILE:HD13	1:A:405:ILE:HD12	1.89	0.54
1:B:225:ILE:HD13	1:B:405:ILE:HD12	1.89	0.54
1:B:69:VAL:HG13	1:B:79:LEU:HD22	1.90	0.53
1:A:69:VAL:HG13	1:A:79:LEU:HD22	1.90	0.53
1:A:304:LYS:HE2	2:D:82:ARG:HH22	1.74	0.53
1:A:404:SER:O	1:A:407:GLN:HG2	2.09	0.53
2:C:100:LEU:HB3	2:C:105:LYS:HZ2	1.73	0.53
2:D:22:GLN:HE21	2:D:26:LYS:HZ1	1.52	0.53
1:B:42:ASN:ND2	1:B:79:LEU:HB3	2.25	0.52
1:A:304:LYS:HE2	2:D:82:ARG:NH2	2.25	0.51
1:A:151:ALA:HB1	1:B:128:LEU:HD23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TRP:CD1	1:A:73:LEU:HD12	2.47	0.50
1:B:45:TRP:CD1	1:B:73:LEU:HD12	2.46	0.50
1:B:182:ILE:HA	1:B:185:ARG:HG2	1.93	0.49
2:D:60:GLU:HB2	2:D:100:LEU:HD11	1.92	0.49
1:B:41:ASP:OD1	1:B:41:ASP:O	2.30	0.49
1:B:435:ILE:HG21	1:B:438:GLN:HE21	1.77	0.49
1:A:42:ASN:ND2	1:A:79:LEU:HB3	2.27	0.49
1:A:252:PRO:HG2	1:A:334:LEU:HD23	1.94	0.48
1:B:179:VAL:O	1:B:182:ILE:HG13	2.13	0.48
1:B:218:LEU:HD22	1:B:224:ILE:HD13	1.95	0.48
2:C:55:GLY:HA3	2:C:90:ILE:CD1	2.43	0.48
1:B:228:ALA:HB3	1:B:234:LYS:HB2	1.96	0.48
2:D:40:PRO:HG2	2:D:43:LEU:HD12	1.95	0.48
1:A:342:LEU:HD11	1:A:361:ILE:HG22	1.96	0.48
1:B:301:LEU:HD22	1:B:307:MET:HE1	1.94	0.48
1:B:367:ALA:HA	1:B:370:LYS:HE2	1.94	0.48
1:B:252:PRO:HG2	1:B:334:LEU:HD23	1.94	0.48
1:B:345:MET:HB2	1:B:361:ILE:HD13	1.96	0.48
2:C:125:ALA:HB2	2:C:150:ALA:HB3	1.96	0.47
1:A:282:ARG:CZ	1:B:440:ASN:OD1	2.62	0.47
1:B:214:LYS:O	1:B:442:PRO:HD2	2.14	0.47
1:B:342:LEU:HD11	1:B:361:ILE:HG22	1.96	0.47
1:A:218:LEU:HD22	1:A:224:ILE:HD13	1.96	0.47
1:B:347:VAL:HB	1:B:357:GLU:HG3	1.96	0.47
1:A:214:LYS:O	1:A:442:PRO:HD2	2.14	0.47
1:A:347:VAL:HB	1:A:357:GLU:HG3	1.96	0.47
1:B:269:MET:HE1	1:B:307:MET:SD	2.55	0.47
1:A:228:ALA:HB3	1:A:234:LYS:HB2	1.97	0.47
2:C:127:VAL:HG22	2:D:72:TYR:HD1	1.79	0.47
2:D:125:ALA:HB2	2:D:150:ALA:HB3	1.96	0.47
1:A:345:MET:HB2	1:A:361:ILE:HD13	1.96	0.46
1:A:269:MET:HE1	1:A:307:MET:SD	2.56	0.46
1:A:243:GLU:O	1:A:247:MET:SD	2.74	0.46
1:A:163:PHE:CE1	1:A:325:ARG:NH1	2.78	0.45
1:A:300:ILE:HD11	2:D:78:LEU:HD21	1.97	0.45
2:D:22:GLN:HG2	2:D:26:LYS:NZ	2.31	0.45
1:B:367:ALA:HA	1:B:370:LYS:HG2	1.98	0.45
2:C:40:PRO:HG2	2:C:43:LEU:HD12	1.99	0.45
1:A:384:ARG:HG2	1:B:400:ARG:HB3	1.99	0.44
2:D:74:ARG:HH11	2:D:94:VAL:HG23	1.82	0.44
2:D:34:GLN:NE2	2:D:84:ASN:ND2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:HB2	1:B:125:GLU:OE1	2.18	0.44
2:C:74:ARG:HH11	2:C:94:VAL:HG23	1.83	0.44
2:C:21:ILE:HG22	2:C:26:LYS:HG3	2.00	0.44
2:D:22:GLN:CG	2:D:26:LYS:NZ	2.80	0.44
2:C:123:HIS:O	2:C:127:VAL:HG23	2.18	0.43
1:B:41:ASP:OD1	1:B:41:ASP:C	2.62	0.43
1:A:234:LYS:HA	1:A:415:ILE:HD12	2.00	0.43
1:B:226:VAL:HB	1:B:379:LEU:HD23	2.00	0.43
2:D:123:HIS:O	2:D:127:VAL:HG23	2.18	0.43
1:B:239:MET:HE1	1:B:255:ILE:HD13	2.01	0.43
2:D:130:ALA:O	2:D:133:ASP:OD2	2.37	0.43
1:B:45:TRP:CD1	1:B:73:LEU:CD1	3.02	0.43
1:A:226:VAL:HB	1:A:379:LEU:HD23	2.00	0.43
1:A:239:MET:HE1	1:A:255:ILE:HD13	2.01	0.43
1:B:207:GLY:HA3	1:B:244:ASN:ND2	2.34	0.43
1:B:32:GLN:HG2	1:B:106:LEU:CD2	2.49	0.43
1:A:257:SER:OG	1:A:260:MET:O	2.37	0.42
1:B:135:VAL:CG2	1:B:165:ILE:HD11	2.48	0.42
1:B:179:VAL:HA	1:B:182:ILE:HG12	2.00	0.42
1:B:234:LYS:HA	1:B:415:ILE:HD12	2.00	0.42
1:A:45:TRP:CD1	1:A:73:LEU:CD1	3.02	0.42
1:B:65:ILE:HG23	1:B:84:LEU:HD21	2.01	0.42
2:C:127:VAL:HG22	2:D:72:TYR:CD1	2.55	0.42
1:B:57:PHE:HB2	1:B:63:ARG:HG2	2.01	0.42
2:C:120:LEU:HD23	2:C:150:ALA:HB2	2.00	0.42
1:A:207:GLY:HA3	1:A:244:ASN:ND2	2.35	0.42
1:A:32:GLN:HG2	1:A:106:LEU:CD2	2.49	0.42
1:A:55:GLN:O	1:A:130:ARG:NH2	2.52	0.42
1:A:65:ILE:HG23	1:A:84:LEU:HD21	2.01	0.41
2:C:34:GLN:HE22	2:C:84:ASN:HD22	1.64	0.41
1:A:57:PHE:HB2	1:A:63:ARG:HG2	2.02	0.41
2:C:130:ALA:O	2:C:133:ASP:OD2	2.38	0.41
2:D:60:GLU:HB3	2:D:100:LEU:HD11	2.02	0.41
1:B:55:GLN:O	1:B:130:ARG:NH2	2.53	0.41
1:A:228:ALA:HB1	1:A:232:MET:HB2	2.02	0.41
1:A:18:VAL:HG13	1:A:22:LYS:HD2	2.01	0.41
1:B:234:LYS:HG2	1:B:379:LEU:HD22	2.03	0.40
1:B:28:LEU:CD1	1:B:62:HIS:CE1	2.98	0.40
2:C:21:ILE:HG23	2:C:26:LYS:HG3	2.03	0.40
1:A:44:ARG:HH22	1:A:114:ALA:H	1.69	0.40
1:A:229:ARG:HH22	1:A:384:ARG:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:MET:HE1	1:B:307:MET:HE1	2.03	0.40
2:C:100:LEU:HB3	2:C:105:LYS:HZ3	1.86	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	448/474 (94%)	439 (98%)	9 (2%)	0	100	100
1	B	445/474 (94%)	432 (97%)	12 (3%)	1 (0%)	43	72
2	C	147/163 (90%)	137 (93%)	6 (4%)	4 (3%)	4	16
2	D	146/163 (90%)	138 (94%)	7 (5%)	1 (1%)	18	48
All	All	1186/1274 (93%)	1146 (97%)	34 (3%)	6 (0%)	24	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	177	LYS
2	C	41	LYS
2	C	98	PRO
2	C	24	HIS
2	C	112	ARG
2	D	112	ARG

5.3.2 Protein sidechains [i](#)

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	383/403 (95%)	372 (97%)	11 (3%)	37	71
1	B	380/403 (94%)	368 (97%)	12 (3%)	34	68
2	C	123/137 (90%)	118 (96%)	5 (4%)	27	61
2	D	123/137 (90%)	116 (94%)	7 (6%)	18	49
All	All	1009/1080 (93%)	974 (96%)	35 (4%)	32	66

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASP
1	A	115	ASN
1	A	179	VAL
1	A	182	ILE
1	A	183	LEU
1	A	229	ARG
1	A	266	MET
1	A	336	LEU
1	A	384	ARG
1	A	401	GLU
1	A	435	ILE
1	B	28	LEU
1	B	60	ARG
1	B	115	ASN
1	B	167	GLU
1	B	179	VAL
1	B	182	ILE
1	B	183	LEU
1	B	229	ARG
1	B	265	ILE
1	B	336	LEU
1	B	384	ARG
1	B	401	GLU
2	C	90	ILE
2	C	112	ARG
2	C	122	GLU
2	C	133	ASP
2	C	148	ARG
2	D	101	TYR
2	D	112	ARG

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Mol	Chain	Res	Type
2	D	115	ASN
2	D	122	GLU
2	D	127	VAL
2	D	133	ASP
2	D	157	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	115	ASN
1	A	278	GLN
1	A	383	ASN
1	A	422	HIS
1	B	42	ASN
1	B	115	ASN
1	B	278	GLN
1	B	383	ASN
1	B	396	ASN
1	B	422	HIS
2	C	24	HIS
2	C	46	GLN
2	C	84	ASN
2	D	22	GLN
2	D	24	HIS
2	D	34	GLN
2	D	84	ASN
2	D	103	GLN
2	D	115	ASN

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 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
3	ADP	A	501	-	28,29,29	0.48	0	43,45,45	0.52	0
3	ADP	B	501	-	28,29,29	0.48	0	43,45,45	0.51	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
3	ADP	A	501	-	-	3/16/32/32	0/3/3/3
3	ADP	B	501	-	-	3/16/32/32	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

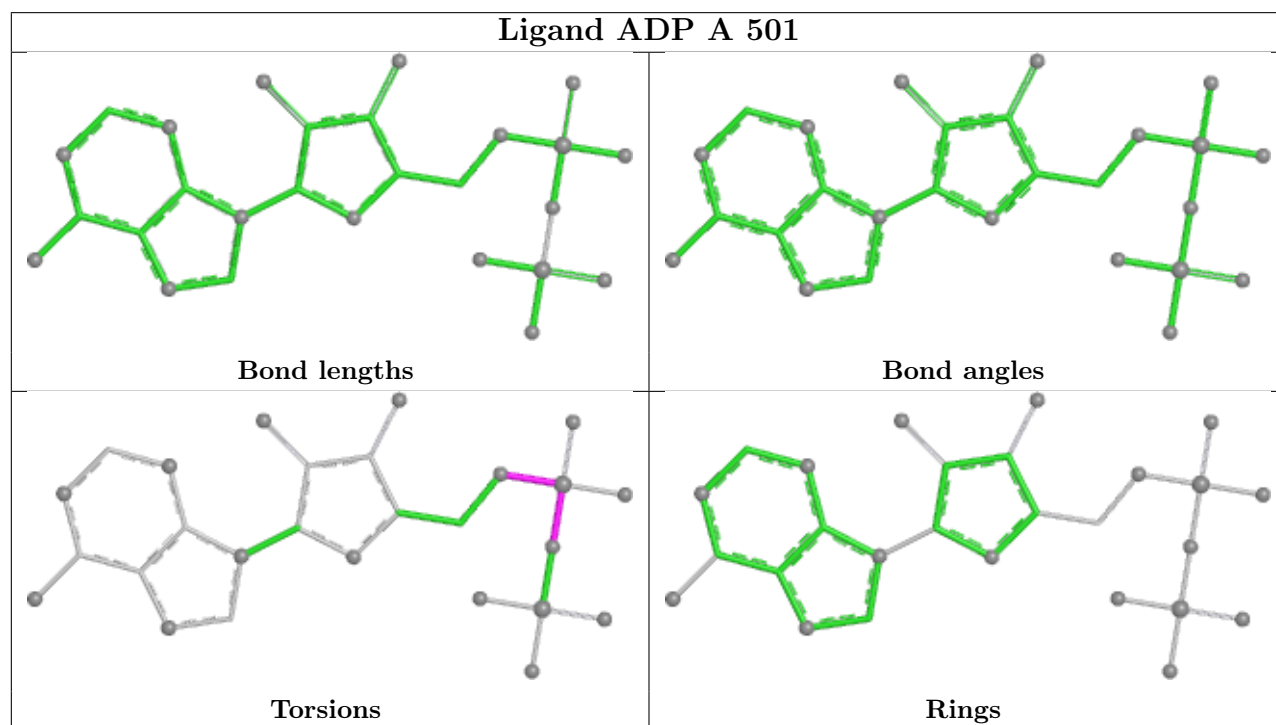
All (6) torsion outliers are listed below:

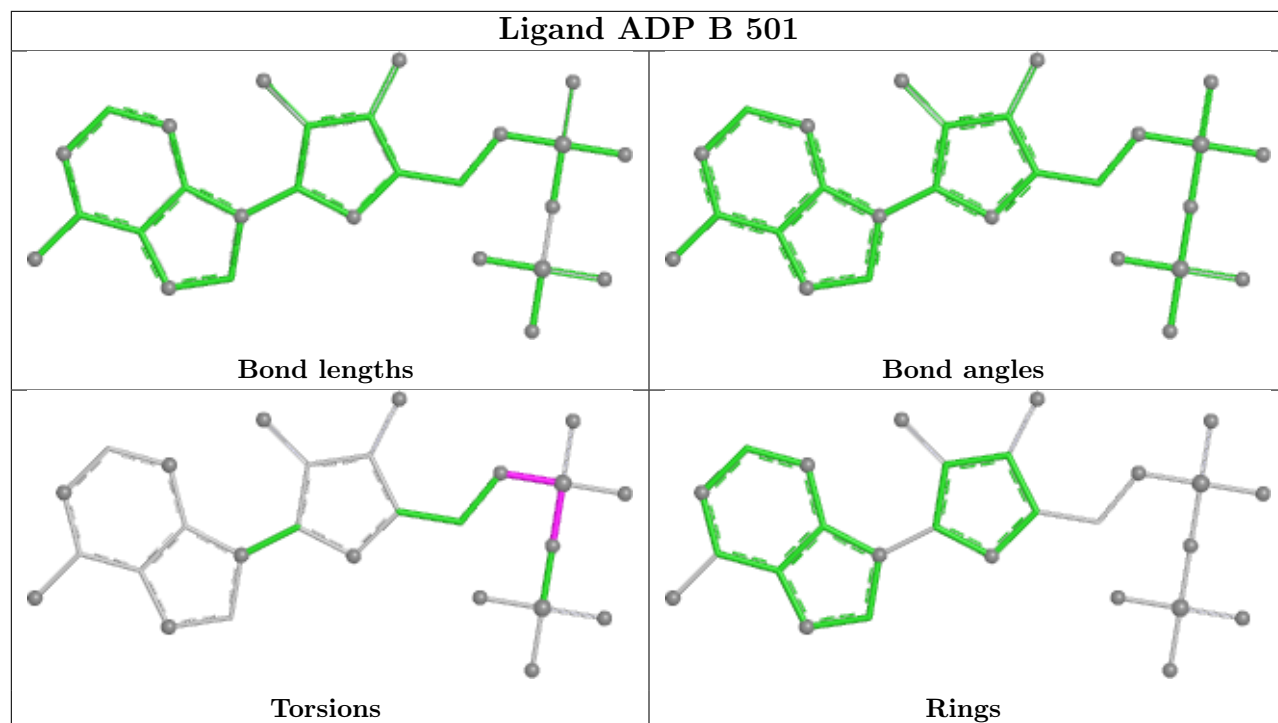
Mol	Chain	Res	Type	Atoms
3	A	501	ADP	C5'-O5'-PA-O2A
3	A	501	ADP	C5'-O5'-PA-O3A
3	B	501	ADP	C5'-O5'-PA-O2A
3	B	501	ADP	C5'-O5'-PA-O3A
3	A	501	ADP	PB-O3A-PA-O2A
3	B	501	ADP	PB-O3A-PA-O2A

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	450/474 (94%)	1.94	179 (39%) 1 0	45, 115, 215, 229	0
1	B	447/474 (94%)	1.99	185 (41%) 0 0	61, 117, 186, 196	0
2	C	149/163 (91%)	2.12	65 (43%) 0 0	115, 136, 203, 209	7 (4%)
2	D	148/163 (90%)	1.69	51 (34%) 1 1	73, 108, 165, 172	0
All	All	1194/1274 (93%)	1.95	480 (40%) 0 0	45, 119, 199, 229	7 (0%)

All (480) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	324	ALA	15.3
1	A	365	LEU	9.8
1	B	241	LEU	8.5
1	B	399	LEU	8.4
2	C	94	VAL	8.3
1	A	327	ILE	8.1
1	B	414	PHE	8.0
1	B	405	ILE	7.5
1	B	377	VAL	7.4
2	C	77	ILE	7.2
1	A	301	LEU	7.0
1	A	342	LEU	6.9
1	B	442	PRO	6.9
1	A	309	ILE	6.8
2	C	59	LEU	6.7
1	A	298	MET	6.6
2	C	125	ALA	6.5
1	A	110	THR	6.3
2	D	149	LEU	6.1
1	B	255	ILE	6.0
1	B	225	ILE	6.0

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Mol	Chain	Res	Type	RSRZ
2	D	124	ALA	6.0
2	C	31	ILE	6.0
1	A	84	LEU	5.9
1	A	291	TRP	5.9
1	A	430	THR	5.9
1	B	325	ARG	5.9
1	B	365	LEU	5.9
1	A	414	PHE	5.8
1	B	411	LEU	5.7
1	A	225	ILE	5.6
1	A	233	GLY	5.6
1	B	416	TYR	5.5
1	A	307	MET	5.4
1	B	378	ALA	5.3
1	B	415	ILE	5.3
1	A	227	ALA	5.3
1	B	358	ILE	5.3
1	A	106	LEU	5.2
1	B	98	GLY	5.2
2	D	132	ALA	5.2
1	B	166	ALA	5.2
1	A	338	MET	5.1
2	D	29	LEU	5.1
1	B	413	MET	5.1
1	A	255	ILE	5.1
1	A	193	LEU	5.0
2	D	104	SER	5.0
1	A	186	THR	5.0
2	C	21	ILE	5.0
2	C	139	VAL	5.0
1	B	224	ILE	4.9
1	B	412	ILE	4.9
2	C	35	LEU	4.9
1	A	362	SER	4.9
2	C	100	LEU	4.9
1	A	378	ALA	4.8
1	A	353	ASN	4.8
1	B	320	VAL	4.8
2	D	153	ASN	4.8
1	A	415	ILE	4.7
1	A	334	LEU	4.7
2	C	39	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	273	LEU	4.7
1	B	396	ASN	4.7
1	B	291	TRP	4.6
1	A	262	ALA	4.6
1	A	407	GLN	4.5
2	D	105	LYS	4.5
1	B	443	ILE	4.5
2	C	29	LEU	4.5
1	A	294	ILE	4.5
1	A	361	ILE	4.5
1	B	122	ILE	4.5
1	B	340	ASP	4.5
2	C	30	LEU	4.5
2	C	131	ILE	4.4
1	A	308	TYR	4.4
1	B	142	ALA	4.4
1	B	183	LEU	4.4
2	D	120	LEU	4.4
1	B	110	THR	4.4
1	A	336	LEU	4.3
1	A	371	GLU	4.3
1	B	230	PRO	4.3
1	B	381	GLN	4.3
2	D	131	ILE	4.2
1	B	25	PRO	4.2
1	B	39	LEU	4.2
1	A	249	GLN	4.2
1	A	381	GLN	4.2
2	C	101	TYR	4.2
1	A	320	VAL	4.2
2	C	43	LEU	4.2
2	D	30	LEU	4.2
2	D	107	THR	4.1
2	D	35	LEU	4.1
1	A	228	ALA	4.1
1	B	341	TYR	4.1
1	B	308	TYR	4.1
1	B	265	ILE	4.1
1	B	364	SER	4.1
1	B	162	VAL	4.0
1	B	75	ALA	4.0
1	B	357	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	15	ASP	4.0
1	B	455	SER	4.0
2	D	108	SER	4.0
1	A	394	PRO	4.0
2	C	27	ALA	4.0
1	A	82	ILE	4.0
1	B	382	LEU	4.0
1	B	246	ALA	3.9
1	B	273	LEU	3.9
2	C	128	LEU	3.9
1	A	377	VAL	3.9
1	A	402	SER	3.9
2	C	47	VAL	3.9
2	C	127	VAL	3.9
1	A	208	PHE	3.9
1	A	358	ILE	3.8
1	A	411	LEU	3.8
1	A	162	VAL	3.8
1	B	349	ALA	3.8
1	B	315	LEU	3.8
1	A	253	VAL	3.8
1	A	337	ILE	3.8
1	B	143	GLY	3.8
1	A	257	SER	3.7
1	A	386	LEU	3.7
1	B	81	LEU	3.7
1	B	309	ILE	3.7
1	B	361	ILE	3.7
1	B	433	ILE	3.7
1	B	344	LEU	3.7
1	B	441	GLY	3.7
1	B	318	THR	3.7
1	A	179	VAL	3.7
1	A	182	ILE	3.7
1	B	175	GLY	3.7
1	B	406	GLU	3.7
1	B	368	LEU	3.6
1	B	310	ASP	3.6
2	C	130	ALA	3.6
2	D	28	ILE	3.6
1	A	356	LEU	3.6
1	B	397	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	380	SER	3.5
1	A	413	MET	3.5
1	A	449	THR	3.5
1	A	183	LEU	3.5
1	B	38	LEU	3.5
2	C	89	LEU	3.5
1	B	180	ASP	3.5
1	B	324	ALA	3.5
1	B	379	LEU	3.5
1	B	321	ARG	3.5
1	A	404	SER	3.4
1	B	380	SER	3.4
1	B	440	ASN	3.4
1	A	223	LEU	3.4
1	B	254	LEU	3.4
1	B	317	PRO	3.4
1	B	66	PHE	3.4
1	B	372	LEU	3.4
2	C	81	LEU	3.4
1	B	33	SER	3.4
1	A	165	ILE	3.4
1	B	79	LEU	3.4
2	C	52	VAL	3.4
1	B	408	ASP	3.4
1	A	241	LEU	3.3
1	B	342	LEU	3.3
1	A	339	VAL	3.3
1	A	446	VAL	3.3
1	A	281	ILE	3.3
1	B	402	SER	3.3
1	A	345	MET	3.3
1	B	409	ALA	3.3
1	A	226	VAL	3.3
1	A	299	GLY	3.3
2	C	106	ILE	3.3
1	A	450	PHE	3.3
1	A	330	GLU	3.3
1	B	174	GLU	3.3
1	A	302	MET	3.3
1	A	224	ILE	3.3
1	A	405	ILE	3.3
1	B	35	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	106	ILE	3.3
1	B	120	ALA	3.3
1	A	270	LEU	3.3
2	C	142	ARG	3.3
1	A	388	GLN	3.3
1	B	337	ILE	3.2
2	C	70	VAL	3.2
1	B	236	THR	3.2
1	A	176	PRO	3.2
1	B	84	LEU	3.2
2	D	111	ALA	3.2
1	B	430	THR	3.2
1	B	58	TYR	3.2
2	D	31	ILE	3.2
1	B	447	ARG	3.2
1	A	265	ILE	3.2
1	A	343	GLN	3.2
1	B	294	ILE	3.2
1	A	211	LEU	3.1
1	B	400	ARG	3.1
2	C	98	PRO	3.1
1	A	368	LEU	3.1
2	C	58	VAL	3.1
1	A	375	PRO	3.1
1	B	389	ARG	3.1
2	C	78	LEU	3.1
1	A	161	LYS	3.1
1	A	341	TYR	3.1
1	B	176	PRO	3.1
1	B	301	LEU	3.1
2	C	24	HIS	3.1
1	B	97	VAL	3.1
2	D	92	ILE	3.1
1	B	34	VAL	3.0
1	B	347	VAL	3.0
1	A	278	GLN	3.0
1	A	382	LEU	3.0
1	B	336	LEU	3.0
1	A	45	TRP	3.0
1	B	446	VAL	3.0
1	A	459	ASN	3.0
1	A	326	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	435	ILE	3.0
1	A	360	GLU	3.0
1	A	359	ALA	3.0
1	B	179	VAL	3.0
1	A	194	TYR	3.0
1	A	295	SER	3.0
1	A	399	LEU	3.0
1	B	103	LEU	3.0
1	B	394	PRO	3.0
2	C	93	GLU	3.0
1	A	367	ALA	3.0
2	D	125	ALA	3.0
2	C	92	ILE	3.0
1	A	81	LEU	3.0
1	A	379	LEU	3.0
1	B	448	LEU	3.0
2	D	89	LEU	3.0
1	A	431	ALA	3.0
1	B	253	VAL	3.0
1	A	286	LEU	2.9
2	D	128	LEU	2.9
1	B	181	SER	2.9
1	B	234	LYS	2.9
1	A	139	ILE	2.9
1	B	132	LEU	2.9
1	B	438	GLN	2.9
1	A	317	PRO	2.9
1	B	362	SER	2.9
1	B	431	ALA	2.9
2	C	124	ALA	2.9
1	B	116	ILE	2.9
2	D	21	ILE	2.9
1	A	192	LEU	2.9
1	A	269	MET	2.9
2	D	27	ALA	2.9
1	A	335	SER	2.9
1	B	62	HIS	2.9
1	B	307	MET	2.8
1	B	398	ASP	2.8
1	B	327	ILE	2.8
1	B	439	ARG	2.8
1	A	157	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	286	LEU	2.8
1	A	429	GLY	2.8
1	A	323	ARG	2.8
1	B	107	ALA	2.8
2	C	86	PHE	2.8
2	D	57	LEU	2.8
1	A	340	ASP	2.8
1	B	47	THR	2.8
1	B	54	THR	2.8
1	A	175	GLY	2.8
1	B	57	PHE	2.8
1	B	94	LEU	2.8
2	D	51	ASN	2.8
1	A	126	ARG	2.7
1	B	339	VAL	2.7
1	A	113	ALA	2.7
1	A	245	ALA	2.7
2	C	141	LYS	2.7
1	A	310	ASP	2.7
2	C	79	THR	2.7
2	D	82	ARG	2.7
1	A	155	LEU	2.7
1	A	266	MET	2.7
1	B	420	VAL	2.7
1	A	103	LEU	2.7
1	A	166	ALA	2.7
1	A	344	LEU	2.7
1	B	190	ILE	2.7
2	C	28	ILE	2.7
1	B	235	THR	2.7
2	D	32	ASN	2.7
1	B	345	MET	2.7
1	B	144	TYR	2.7
2	D	47	VAL	2.7
1	B	404	SER	2.7
1	A	416	TYR	2.6
1	A	348	PRO	2.6
1	A	196	THR	2.6
1	A	311	ASP	2.6
1	A	350	LEU	2.6
2	D	17	LYS	2.6
2	C	54	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	118	PRO	2.6
1	B	281	ILE	2.6
2	D	110	ASP	2.6
1	A	118	ALA	2.6
2	C	102	ARG	2.6
1	A	254	LEU	2.6
1	B	48	VAL	2.6
1	A	256	PHE	2.6
1	B	136	ALA	2.6
2	D	49	ALA	2.6
1	B	453	HIS	2.6
1	A	372	LEU	2.6
2	C	12	LEU	2.6
2	C	45	THR	2.6
2	C	96	VAL	2.6
2	D	156	ASP	2.6
1	A	25	PRO	2.5
2	D	59	LEU	2.5
1	A	300	ILE	2.5
1	A	297	THR	2.5
2	C	23	GLU	2.5
1	A	328	ALA	2.5
2	D	152	ALA	2.5
1	B	187	LEU	2.5
2	D	118	PRO	2.5
1	B	216	ALA	2.5
1	A	354	ARG	2.5
1	A	267	MET	2.5
1	A	190	ILE	2.5
1	B	104	ALA	2.5
2	C	75	LEU	2.5
1	B	237	PHE	2.5
1	A	198	GLN	2.5
1	A	396	ASN	2.5
1	B	154	LEU	2.4
2	C	57	LEU	2.4
1	A	325	ARG	2.4
1	B	149	ARG	2.4
1	A	147	GLN	2.4
2	D	80	GLN	2.4
1	A	154	LEU	2.4
2	D	52	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	93	GLN	2.4
1	B	118	ALA	2.4
1	B	83	THR	2.4
1	B	297	THR	2.4
1	B	65	ILE	2.4
1	A	403	GLY	2.4
1	A	231	SER	2.4
1	A	158	ALA	2.4
2	D	50	ALA	2.4
1	A	73	LEU	2.4
1	A	315	LEU	2.4
1	B	155	LEU	2.4
2	D	70	VAL	2.4
2	C	74	ARG	2.4
1	B	227	ALA	2.4
2	C	147	ALA	2.4
2	D	113	ALA	2.4
1	B	283	THR	2.4
1	A	132	LEU	2.4
2	D	123	HIS	2.4
1	A	293	ARG	2.3
1	B	123	VAL	2.3
1	B	395	VAL	2.3
2	D	150	ALA	2.3
1	B	335	SER	2.3
1	A	72	ILE	2.3
1	B	139	ILE	2.3
1	A	177	LYS	2.3
2	C	105	LYS	2.3
1	B	436	GLY	2.3
1	A	100	PHE	2.3
1	B	46	ASP	2.3
1	B	158	ALA	2.3
2	C	76	HIS	2.3
1	A	133	ILE	2.3
1	A	433	ILE	2.3
1	B	454	TYR	2.3
1	B	375	PRO	2.3
2	D	48	ARG	2.3
1	A	129	VAL	2.3
2	C	99	GLU	2.3
2	C	137	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	146	LEU	2.3
1	A	331	HIS	2.3
1	A	204	VAL	2.3
2	C	85	GLY	2.3
1	A	16	ALA	2.3
1	B	151	ALA	2.3
1	A	448	LEU	2.3
1	B	106	LEU	2.3
2	D	38	ILE	2.3
2	C	107	THR	2.3
1	B	194	TYR	2.3
1	B	421	TYR	2.3
1	A	376	VAL	2.3
1	B	100	PHE	2.2
1	B	457	PHE	2.2
1	A	349	ALA	2.2
2	C	64	ALA	2.2
2	C	34	GLN	2.2
1	B	410	ASP	2.2
1	B	130	ARG	2.2
1	B	186	THR	2.2
1	A	20	ALA	2.2
1	A	79	LEU	2.2
1	B	217	GLY	2.2
2	C	68	MET	2.2
1	A	125	GLU	2.2
1	B	124	ALA	2.2
1	B	82	ILE	2.2
2	C	38	ILE	2.2
1	A	146	PRO	2.2
1	B	146	PRO	2.2
1	B	226	VAL	2.2
1	B	257	SER	2.2
1	B	256	PHE	2.2
1	A	387	GLU	2.2
1	B	140	ALA	2.2
1	A	222	ASP	2.2
1	A	421	TYR	2.2
1	B	160	SER	2.2
2	C	120	LEU	2.2
1	A	86	GLU	2.2
2	D	25	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	PRO	2.1
1	A	444	GLY	2.1
2	D	87	GLY	2.1
1	B	211	LEU	2.1
2	D	18	LEU	2.1
2	D	77	ILE	2.1
1	A	197	PRO	2.1
2	C	129	LEU	2.1
2	D	16	SER	2.1
1	B	278	GLN	2.1
2	D	26	LYS	2.1
2	C	18	LEU	2.1
1	A	235	THR	2.1
1	A	458	ASP	2.1
1	A	292	ALA	2.1
1	B	165	ILE	2.1
1	A	445	SER	2.1
2	C	22	GLN	2.1
1	A	247	MET	2.1
1	A	123	VAL	2.1
1	A	370	LYS	2.1
1	B	150	ASN	2.1
1	B	427	LEU	2.1
2	D	143	LEU	2.1
1	A	329	ARG	2.1
1	B	170	THR	2.1
1	B	417	ARG	2.1
1	B	188	GLU	2.1
1	B	437	LYS	2.0
2	C	80	GLN	2.0
1	A	135	VAL	2.0
1	A	314	GLY	2.0
1	B	329	ARG	2.0
1	A	398	ASP	2.0
1	B	222	ASP	2.0
1	B	418	ASP	2.0
2	C	91	SER	2.0
1	B	21	ILE	2.0
1	B	129	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

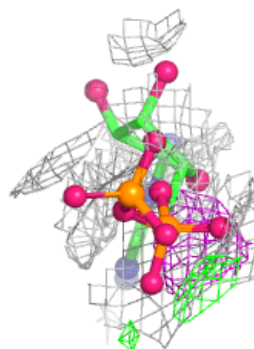
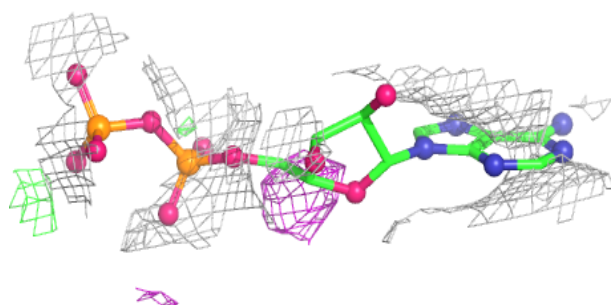
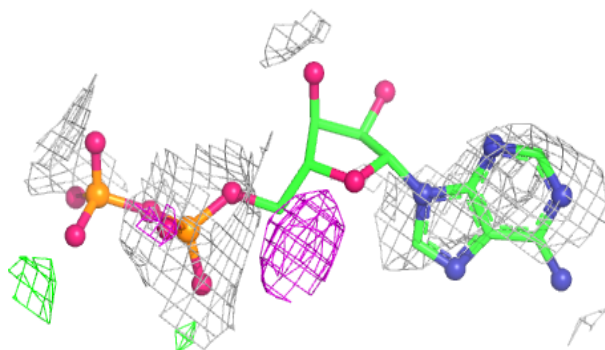
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ADP	B	501	27/27	0.41	0.18	194,195,195,195	0
3	ADP	A	501	27/27	0.83	0.11	71,72,72,72	0
4	MG	A	502	1/1	0.87	0.23	63,63,63,63	0
4	MG	B	502	1/1	0.88	0.28	73,73,73,73	0

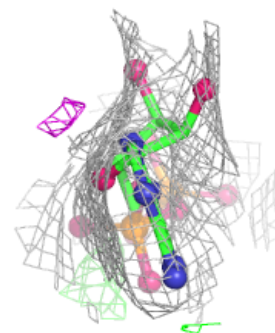
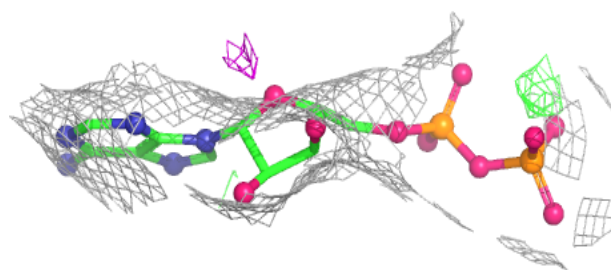
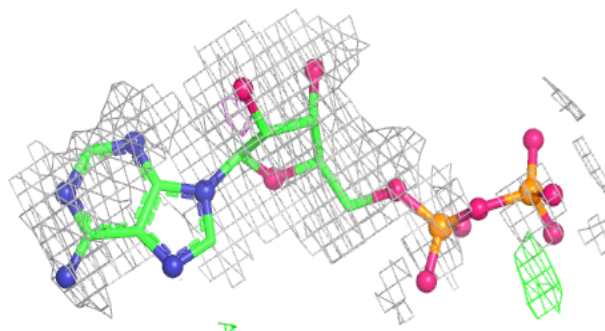
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP B 501:

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

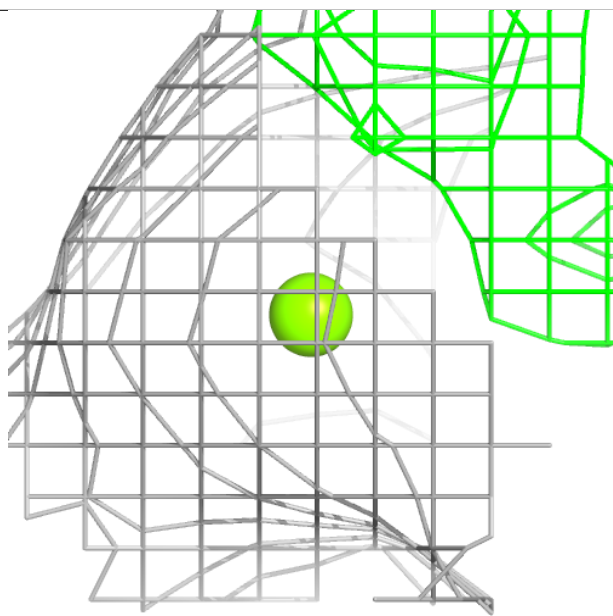
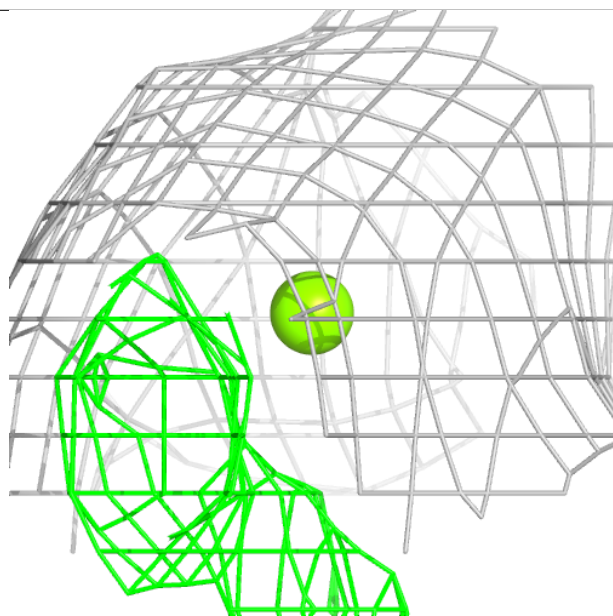
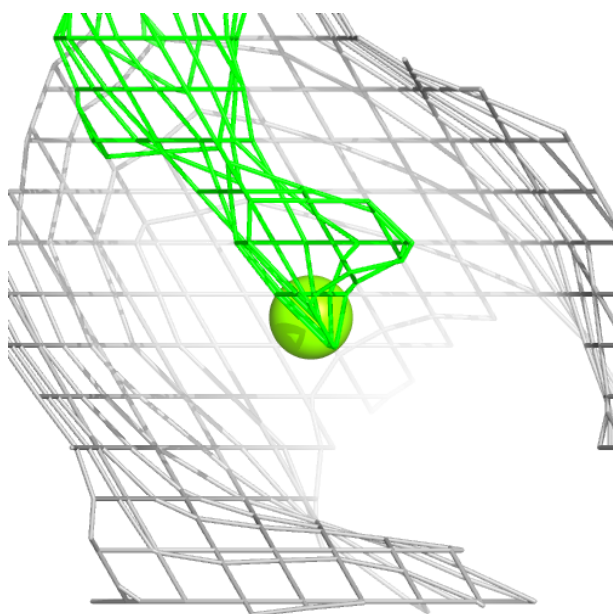
**Electron density around ADP A 501:**

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



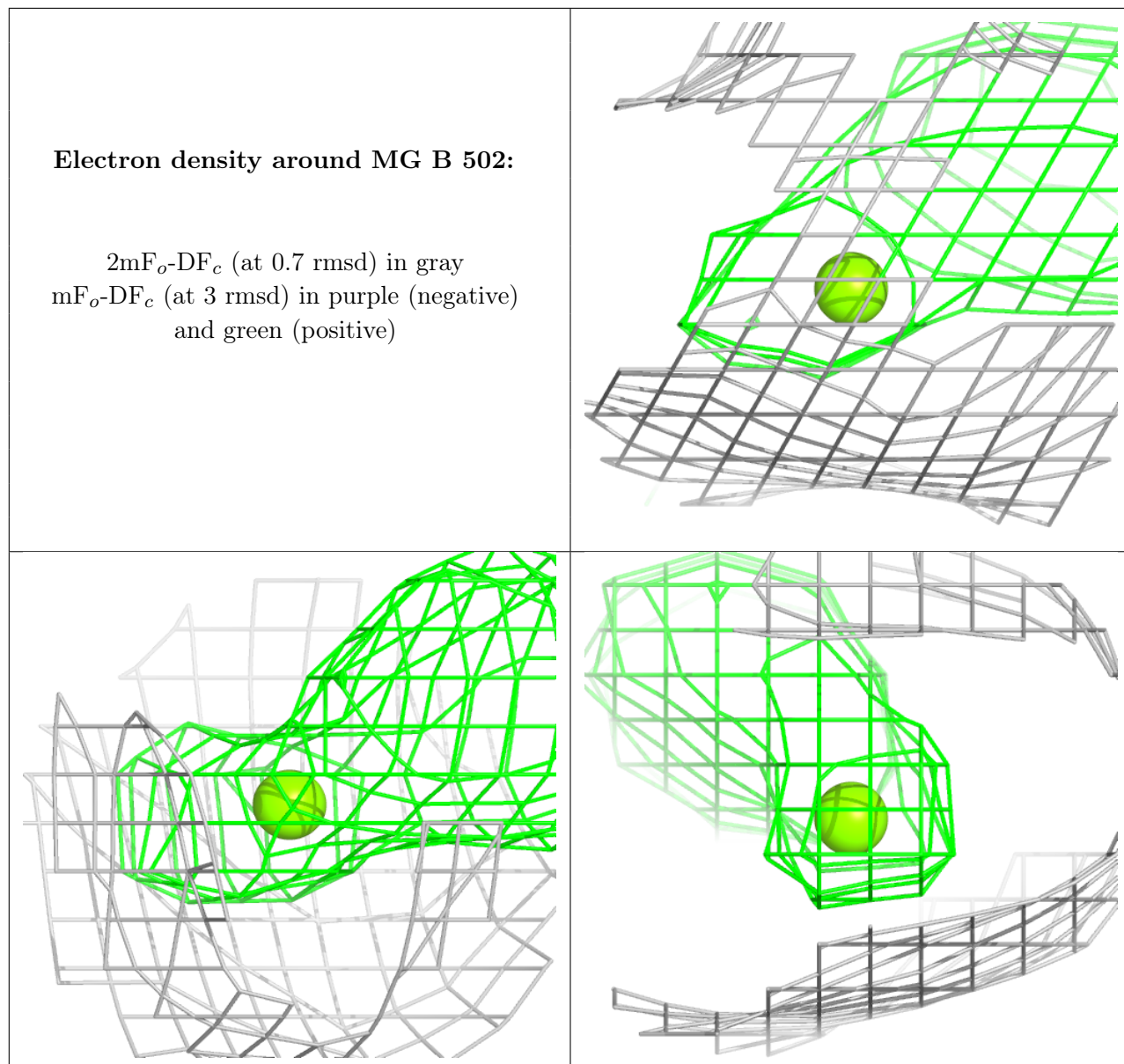
Electron density around MG A 502:

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



Electron density around MG B 502:

$2mF_o-DF_c$ (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.