



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:59 AM UTC

PDB ID : 7CQX / pdb_00007cqx
Title : GmaS/ADP complex-Conformation 2
Authors : Li, C.Y.; Zhang, Y.Z.
Deposited on : 2020-08-11
Resolution : 2.30 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

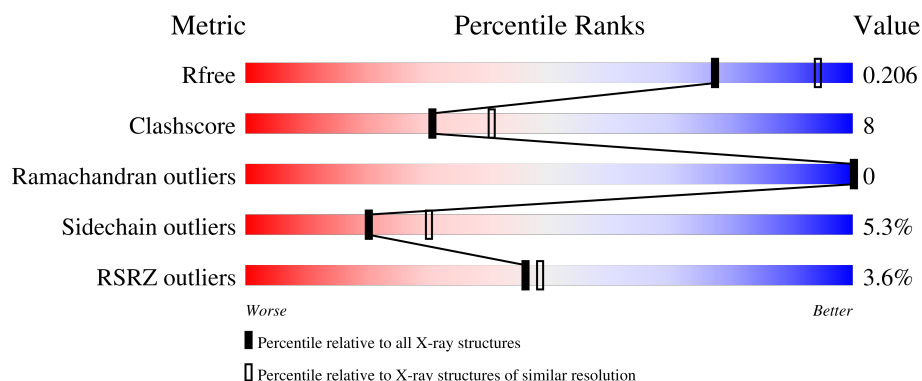
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	450	4% 76% 17% • 6%
1	B	450	3% 76% 16% • 6%
1	C	450	4% 78% 15% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10586 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 Type III glutamate–ammonia ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3221	2046	557	600	18			
1	B	421	Total	C	N	O	S	0	1	0
			3226	2049	557	602	18			
1	C	421	Total	C	N	O	S	0	0	0
			3221	2046	557	600	18			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A369R1N0
A	-18	GLY	-	expression tag	UNP A0A369R1N0
A	-17	SER	-	expression tag	UNP A0A369R1N0
A	-16	SER	-	expression tag	UNP A0A369R1N0
A	-15	HIS	-	expression tag	UNP A0A369R1N0
A	-14	HIS	-	expression tag	UNP A0A369R1N0
A	-13	HIS	-	expression tag	UNP A0A369R1N0
A	-12	HIS	-	expression tag	UNP A0A369R1N0
A	-11	HIS	-	expression tag	UNP A0A369R1N0
A	-10	HIS	-	expression tag	UNP A0A369R1N0
A	-9	SER	-	expression tag	UNP A0A369R1N0
A	-8	SER	-	expression tag	UNP A0A369R1N0
A	-7	GLY	-	expression tag	UNP A0A369R1N0
A	-6	LEU	-	expression tag	UNP A0A369R1N0
A	-5	VAL	-	expression tag	UNP A0A369R1N0
A	-4	PRO	-	expression tag	UNP A0A369R1N0
A	-3	ARG	-	expression tag	UNP A0A369R1N0
A	-2	GLY	-	expression tag	UNP A0A369R1N0
A	-1	SER	-	expression tag	UNP A0A369R1N0
A	0	HIS	-	expression tag	UNP A0A369R1N0
B	-19	MET	-	initiating methionine	UNP A0A369R1N0
B	-18	GLY	-	expression tag	UNP A0A369R1N0
B	-17	SER	-	expression tag	UNP A0A369R1N0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	expression tag	UNP A0A369R1N0
B	-15	HIS	-	expression tag	UNP A0A369R1N0
B	-14	HIS	-	expression tag	UNP A0A369R1N0
B	-13	HIS	-	expression tag	UNP A0A369R1N0
B	-12	HIS	-	expression tag	UNP A0A369R1N0
B	-11	HIS	-	expression tag	UNP A0A369R1N0
B	-10	HIS	-	expression tag	UNP A0A369R1N0
B	-9	SER	-	expression tag	UNP A0A369R1N0
B	-8	SER	-	expression tag	UNP A0A369R1N0
B	-7	GLY	-	expression tag	UNP A0A369R1N0
B	-6	LEU	-	expression tag	UNP A0A369R1N0
B	-5	VAL	-	expression tag	UNP A0A369R1N0
B	-4	PRO	-	expression tag	UNP A0A369R1N0
B	-3	ARG	-	expression tag	UNP A0A369R1N0
B	-2	GLY	-	expression tag	UNP A0A369R1N0
B	-1	SER	-	expression tag	UNP A0A369R1N0
B	0	HIS	-	expression tag	UNP A0A369R1N0
C	-19	MET	-	initiating methionine	UNP A0A369R1N0
C	-18	GLY	-	expression tag	UNP A0A369R1N0
C	-17	SER	-	expression tag	UNP A0A369R1N0
C	-16	SER	-	expression tag	UNP A0A369R1N0
C	-15	HIS	-	expression tag	UNP A0A369R1N0
C	-14	HIS	-	expression tag	UNP A0A369R1N0
C	-13	HIS	-	expression tag	UNP A0A369R1N0
C	-12	HIS	-	expression tag	UNP A0A369R1N0
C	-11	HIS	-	expression tag	UNP A0A369R1N0
C	-10	HIS	-	expression tag	UNP A0A369R1N0
C	-9	SER	-	expression tag	UNP A0A369R1N0
C	-8	SER	-	expression tag	UNP A0A369R1N0
C	-7	GLY	-	expression tag	UNP A0A369R1N0
C	-6	LEU	-	expression tag	UNP A0A369R1N0
C	-5	VAL	-	expression tag	UNP A0A369R1N0
C	-4	PRO	-	expression tag	UNP A0A369R1N0
C	-3	ARG	-	expression tag	UNP A0A369R1N0
C	-2	GLY	-	expression tag	UNP A0A369R1N0
C	-1	SER	-	expression tag	UNP A0A369R1N0
C	0	HIS	-	expression tag	UNP A0A369R1N0

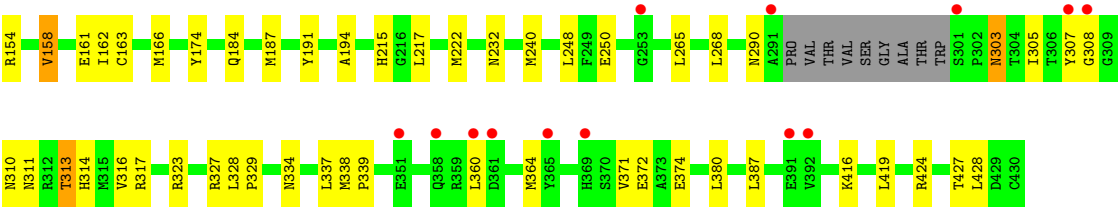
- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	264	Total	O	0	0
			264	264		
3	B	303	Total	O	0	0
			303	303		
3	C	270	Total	O	0	0
			270	270		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	113.45Å 177.56Å 190.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.30 48.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.5 (48.74-2.30) 99.9 (48.74-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.176 , 0.211 0.173 , 0.206	Depositor DCC
R_{free} test set	4091 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10586	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/3301	0.77	0/4486
1	B	0.49	0/3309	0.77	0/4497
1	C	0.48	0/3301	0.78	0/4486
All	All	0.48	0/9911	0.77	0/13469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3221	0	3132	54	0
1	B	3226	0	3136	65	0
1	C	3221	0	3132	45	0
2	A	27	0	11	1	0
2	B	27	0	12	2	0
2	C	27	0	12	4	0
3	A	264	0	0	4	1
3	B	303	0	0	5	0
3	C	270	0	0	5	0
All	All	10586	0	9435	159	1

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 (159) 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:B:338:MET:HG3	1:B:339:PRO:HD3	1.22	1.10
1:A:338:MET:HG3	1:A:339:PRO:HD3	1.31	1.10
1:B:313:THR:HG21	1:B:364:MET:H	1.32	0.94
1:B:313:THR:CG2	1:B:364:MET:H	1.82	0.93
1:B:338:MET:HG3	1:B:339:PRO:CD	2.01	0.90
1:A:338:MET:HG3	1:A:339:PRO:CD	2.09	0.83
1:C:327:ARG:HD2	3:C:611:HOH:O	1.78	0.83
1:A:301:SER:HB3	1:A:302:PRO:HD3	1.59	0.83
1:B:166:MET:HE1	1:B:187:MET:HE2	1.65	0.78
1:A:313:THR:HG21	1:A:364:MET:H	1.48	0.76
1:A:313:THR:CG2	1:A:364:MET:H	1.99	0.75
1:B:301:SER:HB3	1:B:302:PRO:HD3	1.68	0.75
1:C:136:SER:HB2	1:C:217:LEU:HD22	1.68	0.74
1:B:311:ASN:OD1	1:B:313:THR:HB	1.88	0.73
1:A:150:ASP:OD2	3:A:601:HOH:O	2.08	0.72
1:A:1:MET:HE2	1:A:69:PRO:HB2	1.73	0.71
1:B:163:CYS:HA	1:B:166:MET:HE3	1.72	0.70
2:C:500:ADP:O2B	3:C:601:HOH:O	2.09	0.69
1:A:405:ALA:O	1:A:409:ARG:HG3	1.92	0.69
1:A:334:ASN:HB3	1:A:337:LEU:HB2	1.74	0.68
1:B:334:ASN:HB3	1:B:337:LEU:HB2	1.78	0.66
1:C:115:MET:HB3	1:C:240:MET:HE3	1.78	0.65
1:A:184:GLN:HE21	1:A:232:ASN:HD22	1.43	0.65
1:A:53:TRP:CZ2	1:B:144:LYS:HG3	2.32	0.65
1:C:334:ASN:HB3	1:C:337:LEU:HB2	1.78	0.63
1:B:303:ASN:C	1:B:303:ASN:HD22	2.07	0.62
1:A:184:GLN:HE21	1:A:232:ASN:ND2	1.97	0.61
1:A:30:LYS:HE3	1:B:175:GLN:OE1	1.99	0.61
1:C:1:MET:HE3	1:C:2:THR:O	1.99	0.61
1:B:1:MET:HE3	1:B:2:THR:O	2.02	0.60
1:C:119:HIS:HD2	1:C:194:ALA:HA	1.66	0.60
1:C:313:THR:HG21	1:C:364:MET:H	1.66	0.59
1:B:166:MET:CE	1:B:187:MET:HE2	2.32	0.59
1:A:29:ALA:HB2	1:B:149:GLN:HE21	1.66	0.59
1:B:162:ILE:HG22	1:B:166:MET:HE2	1.85	0.59
1:A:313:THR:HG22	1:A:314:HIS:CD2	2.36	0.59
1:C:303:ASN:C	1:C:303:ASN:HD22	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:TRP:CZ2	1:B:416:LYS:HD2	2.38	0.59
1:C:63:ILE:HD13	1:C:88:VAL:HG13	1.83	0.58
1:C:313:THR:HG22	1:C:314:HIS:CD2	2.38	0.58
1:B:161:GLU:OE1	1:B:215:HIS:HE1	1.86	0.58
1:B:119:HIS:HD2	1:B:194:ALA:HA	1.68	0.57
1:B:100:ARG:O	1:B:104:LYS:HG3	2.05	0.57
1:C:360:LEU:HD21	1:C:371:VAL:HG11	1.86	0.56
1:A:119:HIS:CD2	1:A:194:ALA:HA	2.40	0.56
1:B:313:THR:HG21	1:B:364:MET:N	2.11	0.56
1:B:313:THR:HG23	1:B:364:MET:HB2	1.86	0.56
1:C:137:ASP:OD2	1:C:154:ARG:HD2	2.05	0.56
1:A:30:LYS:CE	1:B:175:GLN:OE1	2.52	0.56
1:C:162:ILE:HG22	1:C:166:MET:HE2	1.88	0.56
1:B:115:MET:HB3	1:B:240:MET:HE3	1.87	0.56
1:B:305:ILE:HD12	1:B:374:GLU:HB3	1.88	0.56
1:A:323:ARG:HD3	2:A:500:ADP:C5	2.41	0.56
1:A:119:HIS:HD2	1:A:194:ALA:HA	1.71	0.55
1:C:119:HIS:CD2	1:C:194:ALA:HA	2.41	0.55
1:C:184:GLN:HE21	1:C:232:ASN:HD22	1.54	0.55
1:C:184:GLN:HE21	1:C:232:ASN:ND2	2.05	0.54
1:A:1:MET:HE3	1:A:2:THR:O	2.07	0.54
1:B:405:ALA:O	1:B:409:ARG:HG3	2.06	0.54
1:C:305:ILE:HD12	1:C:374:GLU:HB3	1.89	0.54
1:C:313:THR:CG2	1:C:364:MET:H	2.21	0.54
1:B:63:ILE:HD13	1:B:88:VAL:HG13	1.89	0.54
1:C:323:ARG:HD3	2:C:500:ADP:C5	2.42	0.54
1:A:100:ARG:O	1:A:104:LYS:HG3	2.08	0.54
1:B:136:SER:HB2	1:B:217:LEU:HD22	1.90	0.54
1:C:328:LEU:H	1:C:329:PRO:CD	2.21	0.54
1:B:119:HIS:CD2	1:B:194:ALA:HA	2.43	0.53
1:C:163:CYS:HA	1:C:166:MET:HE3	1.91	0.53
1:B:163:CYS:HA	1:B:166:MET:CE	2.39	0.53
1:A:301:SER:HB3	1:A:302:PRO:CD	2.35	0.53
1:A:312:ARG:NH1	3:A:606:HOH:O	2.42	0.52
1:B:184:GLN:HE21	1:B:232:ASN:ND2	2.08	0.52
1:B:3:ASP:N	1:B:3:ASP:OD1	2.43	0.51
1:C:328:LEU:N	1:C:329:PRO:CD	2.74	0.51
1:B:184:GLN:HE21	1:B:232:ASN:HD22	1.58	0.51
1:A:63:ILE:HD13	1:A:88:VAL:HG13	1.94	0.50
1:A:119:HIS:HA	1:A:237:HIS:O	2.11	0.50
1:C:30:LYS:HG2	1:C:32:VAL:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:TYR:OH	2:C:500:ADP:H3'	2.12	0.50
1:A:23:LEU:HD12	1:A:337:LEU:HD11	1.94	0.49
1:A:95:PHE:CE2	1:A:97:LYS:HB2	2.47	0.49
1:A:136:SER:HB2	1:A:217:LEU:HD22	1.94	0.49
1:B:328:LEU:H	1:B:329:PRO:HD3	1.78	0.49
1:C:328:LEU:H	1:C:329:PRO:HD3	1.78	0.48
1:B:10:GLU:HG3	1:B:11:LYS:HG2	1.95	0.48
1:B:113:LYS:NZ	1:B:351:GLU:OE2	2.46	0.48
1:A:348:ASP:CG	1:A:392:VAL:HG11	2.39	0.48
1:C:310:ASN:OD1	1:C:317:ARG:NH1	2.47	0.48
1:B:313:THR:HG23	1:B:364:MET:H	1.70	0.47
1:A:416:LYS:NZ	3:A:608:HOH:O	2.43	0.47
1:A:313:THR:HG21	1:A:363:ASP:HA	1.97	0.47
1:A:317:ARG:O	1:A:319:PRO:HD3	2.15	0.47
1:B:250:GLU:HG3	3:B:797:HOH:O	2.15	0.47
1:B:290:ASN:O	1:B:291:ALA:C	2.58	0.47
1:A:66:ILE:HA	1:A:67:PRO:HD3	1.79	0.47
1:B:50:PHE:HA	3:B:633:HOH:O	2.14	0.47
1:A:161:GLU:OE1	1:A:215:HIS:HE1	1.97	0.47
1:A:424:ARG:O	1:A:428:LEU:HB2	2.15	0.47
1:B:265:LEU:HD13	1:B:316:VAL:HG11	1.97	0.46
1:B:336:TYR:C	1:B:339:PRO:HD2	2.41	0.46
1:A:311:ASN:OD1	1:A:313:THR:HB	2.16	0.46
1:C:95:PHE:CE2	1:C:97:LYS:HB2	2.50	0.46
1:A:313:THR:HG23	1:A:364:MET:H	1.79	0.45
1:C:161:GLU:OE1	1:C:215:HIS:HE1	1.99	0.45
1:B:191:TYR:HB3	2:B:500:ADP:H1'	1.98	0.45
1:A:247:ASN:OD1	1:A:249:PHE:HB2	2.16	0.45
1:B:336:TYR:O	1:B:339:PRO:HD2	2.16	0.45
1:B:161:GLU:OE1	1:B:215:HIS:CE1	2.69	0.45
1:C:313:THR:HG23	1:C:364:MET:HG2	1.97	0.45
1:A:336:TYR:O	1:A:339:PRO:HD2	2.17	0.45
1:C:372:GLU:OE2	1:C:372:GLU:HA	2.17	0.45
1:B:334:ASN:CB	1:B:337:LEU:HB2	2.46	0.45
1:C:265:LEU:HD13	1:C:316:VAL:HG11	1.99	0.45
1:C:311:ASN:OD1	1:C:313:THR:HG22	2.16	0.45
1:B:301:SER:HB3	1:B:302:PRO:CD	2.41	0.45
1:A:239:SER:HA	1:A:249:PHE:CD2	2.52	0.44
1:B:328:LEU:N	1:B:329:PRO:CD	2.80	0.44
1:B:428:LEU:HD13	1:C:222:MET:SD	2.57	0.44
1:B:24:LEU:HD21	3:B:695:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:TYR:HB2	1:A:308:GLY:HA3	1.99	0.44
1:C:158:VAL:HG12	3:C:827:HOH:O	2.17	0.44
1:A:271:HIS:O	1:A:275:LEU:HB2	2.18	0.44
1:B:124:GLU:HG2	1:B:179:GLU:HG3	2.00	0.44
1:B:424:ARG:O	1:B:428:LEU:HB2	2.18	0.44
1:C:290:ASN:ND2	3:C:607:HOH:O	2.50	0.43
1:C:307:TYR:HB2	1:C:308:GLY:HA3	2.00	0.43
1:A:115:MET:HB3	1:A:240:MET:HE3	2.00	0.43
1:B:313:THR:HG23	1:B:364:MET:CB	2.48	0.43
1:C:100:ARG:O	1:C:104:LYS:HG3	2.18	0.43
1:A:280:ASN:HB3	1:A:285:SER:HB3	2.01	0.43
1:A:290:ASN:O	1:A:291:ALA:C	2.61	0.43
1:C:166:MET:HE1	1:C:187:MET:HE2	2.00	0.43
1:A:162:ILE:HG22	1:A:166:MET:HE2	2.00	0.42
1:C:68:ASP:HB2	3:C:753:HOH:O	2.19	0.42
1:A:62:ASP:OD1	1:B:312:ARG:NH1	2.52	0.42
1:A:313:THR:HG21	1:A:364:MET:N	2.26	0.42
1:B:328:LEU:H	1:B:329:PRO:CD	2.31	0.42
1:B:313:THR:HG21	1:B:363:ASP:HA	2.00	0.42
1:C:23:LEU:HB2	1:C:53:TRP:O	2.19	0.42
1:C:313:THR:CG2	1:C:314:HIS:CD2	3.03	0.42
1:A:166:MET:CE	1:A:187:MET:HE2	2.49	0.42
1:B:63:ILE:C	1:B:63:ILE:HD12	2.45	0.42
1:C:68:ASP:HA	1:C:69:PRO:HD2	1.93	0.42
1:B:119:HIS:HE1	3:B:648:HOH:O	2.03	0.42
1:A:47:PHE:HB2	1:A:63:ILE:HD11	2.01	0.41
1:C:18:ILE:O	1:C:29:ALA:HA	2.20	0.41
1:B:326:LEU:HG	1:B:329:PRO:HD3	2.02	0.41
1:A:328:LEU:N	1:A:329:PRO:CD	2.83	0.41
1:A:110:ALA:HB2	1:A:347:LEU:HD11	2.02	0.41
1:B:66:ILE:HA	1:B:67:PRO:HD3	1.86	0.41
1:B:236:THR:OG1	1:B:338:MET:HE1	2.20	0.41
1:A:309:GLY:O	1:A:317:ARG:HG3	2.21	0.41
1:B:24:LEU:HD22	1:B:53:TRP:CE2	2.56	0.41
1:A:119:HIS:HE1	3:A:736:HOH:O	2.02	0.41
1:B:142:GLN:NE2	3:B:620:HOH:O	2.54	0.41
1:B:323:ARG:HD3	2:B:500:ADP:C5	2.56	0.41
1:C:191:TYR:HB3	2:C:500:ADP:H1'	2.03	0.41
1:B:3:ASP:OD1	1:B:6:SER:HB2	2.21	0.40
1:C:338:MET:HG2	1:C:339:PRO:N	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:789:HOH:O	3:A:834:HOH:O[2_555]	2.19	0.01

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	417/450 (93%)	409 (98%)	8 (2%)	0	100	100
1	B	418/450 (93%)	409 (98%)	9 (2%)	0	100	100
1	C	417/450 (93%)	407 (98%)	10 (2%)	0	100	100
All	All	1252/1350 (93%)	1225 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	324/348 (93%)	308 (95%)	16 (5%)	22	34
1	B	325/348 (93%)	306 (94%)	19 (6%)	18	26
1	C	324/348 (93%)	307 (95%)	17 (5%)	21	31
All	All	973/1044 (93%)	921 (95%)	52 (5%)	20	30

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	32	VAL
1	A	248	LEU
1	A	250	GLU
1	A	268	LEU
1	A	303	ASN
1	A	313	THR
1	A	320	ASP
1	A	338	MET
1	A	360	LEU
1	A	380	LEU
1	A	387	LEU
1	A	416	LYS
1	A	419	LEU
1	A	424	ARG
1	A	428	LEU
1	B	23	LEU
1	B	32	VAL
1	B	123	CYS
1	B	158	VAL
1	B	248	LEU
1	B	250	GLU
1	B	257	LEU
1	B	268	LEU
1	B	303	ASN
1	B	313	THR
1	B	337	LEU
1	B	338	MET
1	B	360	LEU
1	B	380	LEU
1	B	387	LEU
1	B	408	LYS
1	B	416	LYS
1	B	419	LEU
1	B	428	LEU
1	C	23	LEU
1	C	30	LYS
1	C	32	VAL
1	C	123	CYS
1	C	158	VAL
1	C	248	LEU
1	C	250	GLU
1	C	268	LEU

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Mol	Chain	Res	Type
1	C	303	ASN
1	C	313	THR
1	C	380	LEU
1	C	387	LEU
1	C	416	LYS
1	C	419	LEU
1	C	424	ARG
1	C	427	THR
1	C	428	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	ASN
1	A	119	HIS
1	A	182	ASN
1	A	184	GLN
1	A	280	ASN
1	A	290	ASN
1	A	303	ASN
1	A	375	GLN
1	B	119	HIS
1	B	142	GLN
1	B	149	GLN
1	B	182	ASN
1	B	215	HIS
1	B	232	ASN
1	B	290	ASN
1	B	303	ASN
1	B	369	HIS
1	C	119	HIS
1	C	142	GLN
1	C	176	ASN
1	C	182	ASN
1	C	215	HIS
1	C	232	ASN
1	C	290	ASN
1	C	303	ASN
1	C	353	GLN
1	C	375	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	500	-	28,29,29	1.70	5 (17%)	43,45,45	2.06	12 (27%)
2	ADP	C	500	-	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)
2	ADP	B	500	-	28,29,29	1.40	4 (14%)	43,45,45	1.81	9 (20%)

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	ADP	A	500	-	-	2/16/32/32	0/3/3/3
2	ADP	C	500	-	-	3/16/32/32	0/3/3/3
2	ADP	B	500	-	-	2/16/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	ADP	C6-N6	5.62	1.48	1.34
2	B	500	ADP	C5-C4	4.63	1.47	1.39
2	C	500	ADP	C5-C4	4.60	1.47	1.39
2	A	500	ADP	O2'-C2'	-3.07	1.35	1.43
2	C	500	ADP	C5-C6	2.76	1.48	1.41
2	B	500	ADP	C5-C6	2.73	1.48	1.41
2	C	500	ADP	C8-N7	2.35	1.36	1.31
2	B	500	ADP	C8-N7	2.35	1.36	1.31
2	C	500	ADP	C5-N7	-2.26	1.35	1.39
2	B	500	ADP	C5-N7	-2.21	1.35	1.39
2	A	500	ADP	C5-N7	-2.16	1.35	1.39
2	A	500	ADP	O3'-C3'	-2.15	1.37	1.43
2	A	500	ADP	C5'-C4'	-2.01	1.45	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	ADP	C5-C4-N3	-5.71	118.86	126.72
2	B	500	ADP	C5-C4-N3	-5.69	118.88	126.72
2	A	500	ADP	C4-N9-C8	4.74	110.72	105.74
2	A	500	ADP	C5-C4-N3	-4.73	120.21	126.72
2	A	500	ADP	N9-C8-N7	-4.70	107.26	113.94
2	A	500	ADP	N3-C2-N1	-4.63	121.57	128.58
2	C	500	ADP	N3-C4-N9	4.49	134.80	127.17
2	B	500	ADP	N3-C4-N9	4.48	134.79	127.17
2	A	500	ADP	N3-C4-N9	4.32	134.51	127.17
2	C	500	ADP	C2-N3-C4	3.70	120.86	111.83
2	B	500	ADP	C2-N3-C4	3.68	120.81	111.83
2	B	500	ADP	C4-C5-N7	-3.52	106.56	110.58
2	C	500	ADP	C4-C5-N7	-3.49	106.59	110.58
2	A	500	ADP	C5-N7-C8	3.43	108.85	103.45
2	B	500	ADP	N3-C2-N1	-3.29	123.60	128.58
2	C	500	ADP	N3-C2-N1	-3.29	123.60	128.58
2	A	500	ADP	C2-N3-C4	3.19	119.63	111.83
2	B	500	ADP	C4-N9-C8	2.76	108.64	105.74
2	C	500	ADP	C4-N9-C8	2.69	108.56	105.74
2	B	500	ADP	C5-N7-C8	2.56	107.47	103.45
2	C	500	ADP	C5-N7-C8	2.55	107.46	103.45
2	A	500	ADP	O4'-C1'-N9	2.49	112.88	108.09
2	A	500	ADP	C4-C5-N7	-2.35	107.90	110.58
2	B	500	ADP	C6-C5-N7	2.18	136.30	132.09
2	C	500	ADP	C6-C5-N7	2.16	136.25	132.09
2	A	500	ADP	O2A-PA-O3A	2.14	113.06	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	N9-C8-N7	-2.07	111.00	113.94
2	C	500	ADP	N9-C8-N7	-2.04	111.04	113.94
2	A	500	ADP	C5'-C4'-C3'	-2.02	107.94	115.21
2	A	500	ADP	O3B-PB-O3A	2.01	111.39	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

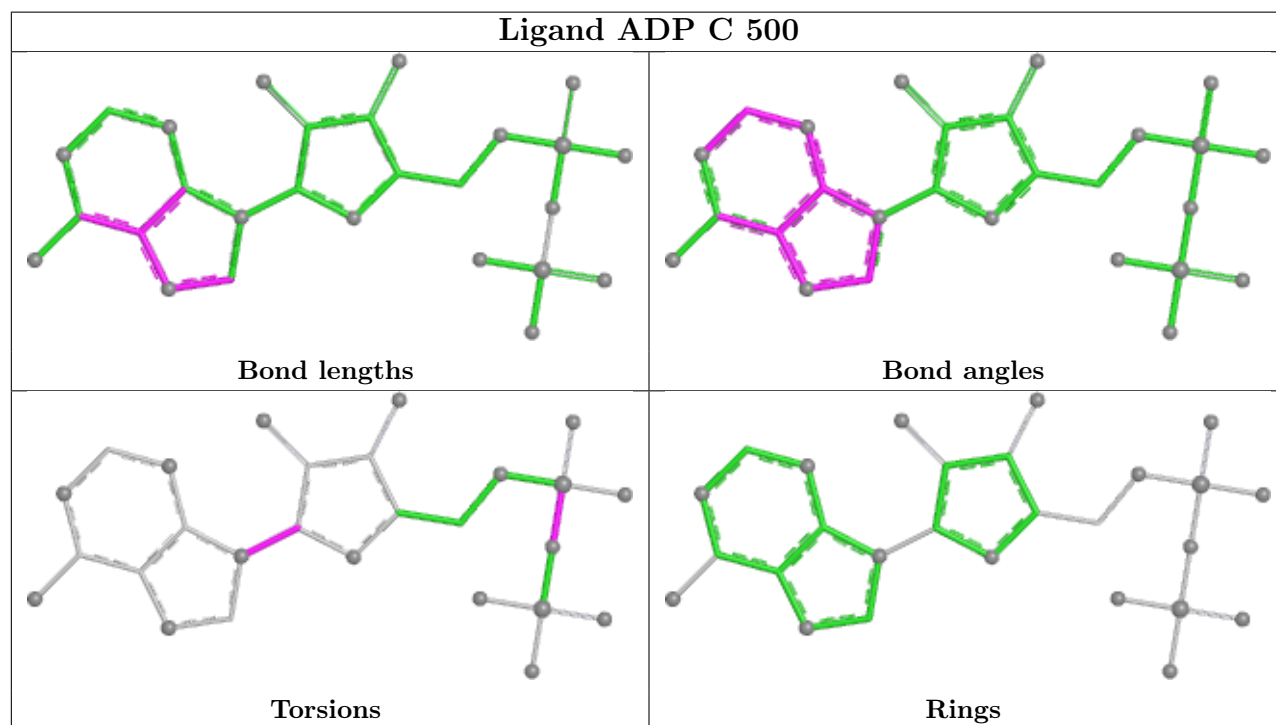
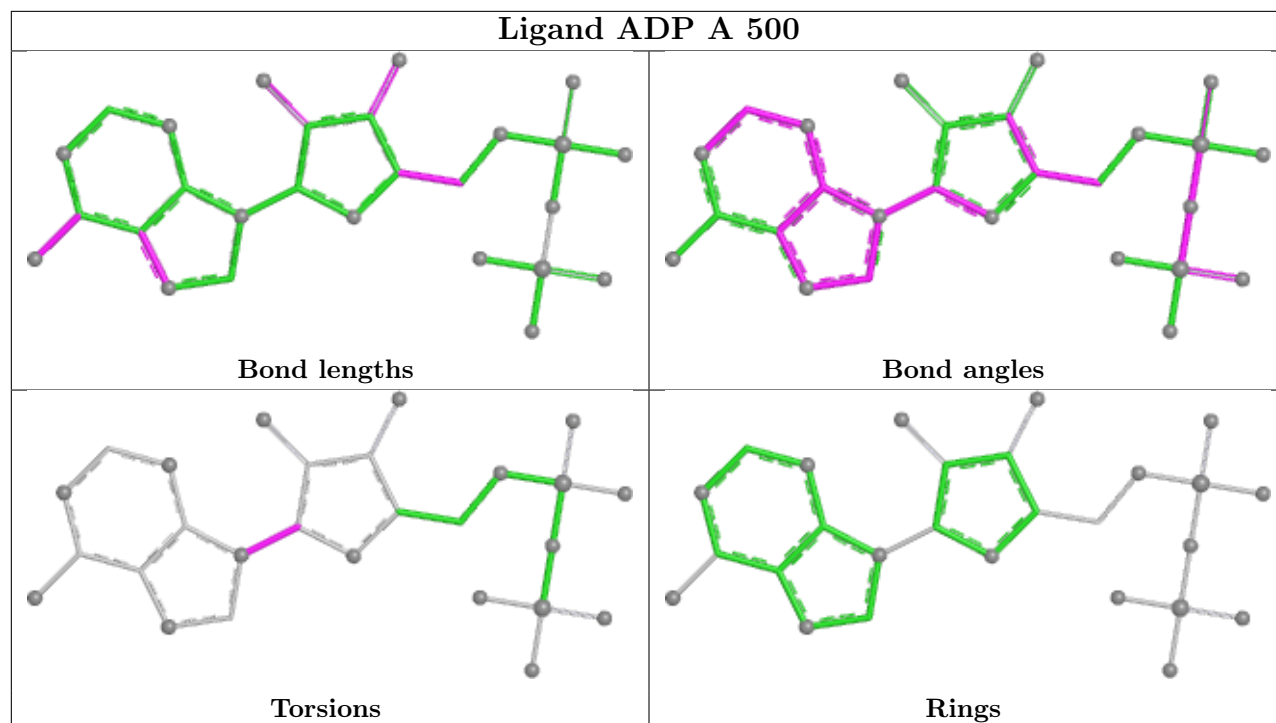
Mol	Chain	Res	Type	Atoms
2	A	500	ADP	C2'-C1'-N9-C8
2	B	500	ADP	C2'-C1'-N9-C8
2	B	500	ADP	PA-O3A-PB-O1B
2	C	500	ADP	C2'-C1'-N9-C8
2	A	500	ADP	O4'-C1'-N9-C8
2	C	500	ADP	PB-O3A-PA-O1A
2	C	500	ADP	PB-O3A-PA-O2A

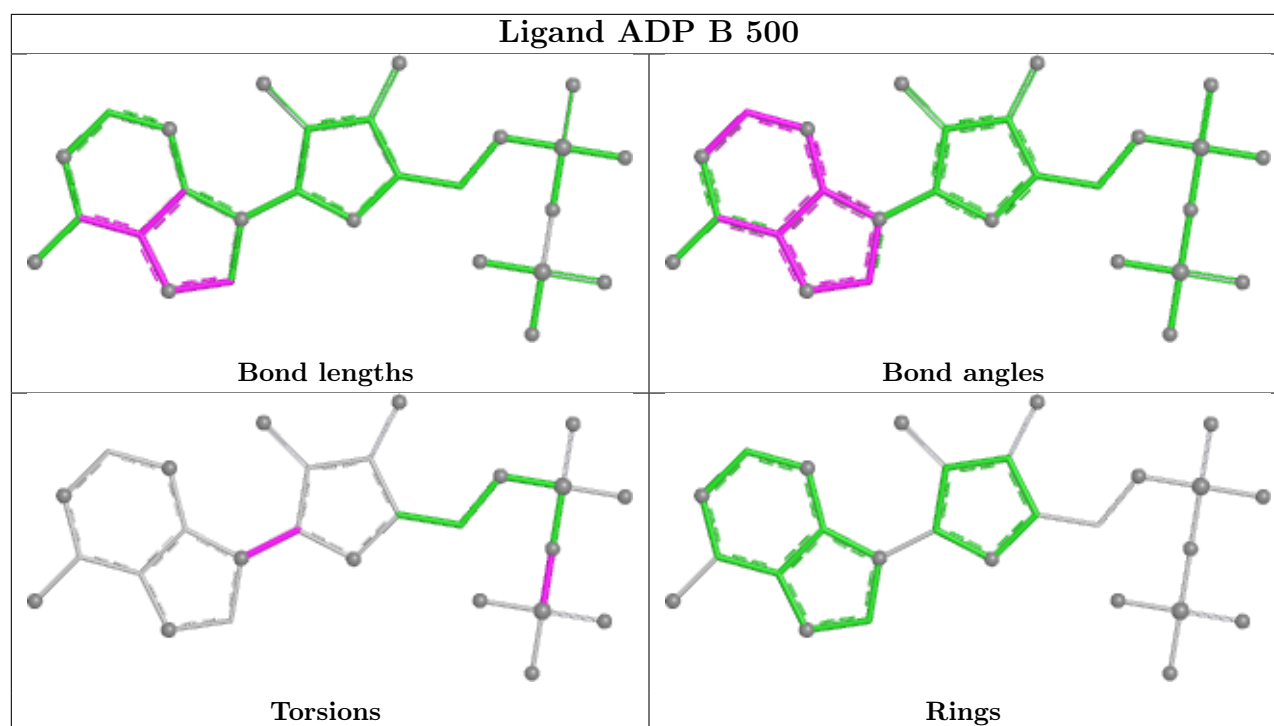
There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ADP	1	0
2	C	500	ADP	4	0
2	B	500	ADP	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	421/450 (93%)	-0.05	16 (3%) 44 46	16, 25, 47, 77	0
1	B	421/450 (93%)	-0.16	13 (3%) 51 53	15, 22, 40, 85	1 (0%)
1	C	421/450 (93%)	-0.05	16 (3%) 44 46	16, 24, 47, 86	0
All	All	1263/1350 (93%)	-0.09	45 (3%) 46 48	15, 24, 46, 86	1 (0%)

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	6.6
1	A	2	THR	5.7
1	B	1	MET	5.6
1	A	1	MET	4.3
1	B	2	THR	4.1
1	B	365	TYR	4.0
1	C	308	GLY	3.5
1	C	2	THR	3.3
1	A	291	ALA	3.3
1	A	368	GLY	3.1
1	C	301	SER	3.0
1	C	391	GLU	2.9
1	C	369	HIS	2.9
1	B	9	ARG	2.8
1	A	308	GLY	2.7
1	A	301	SER	2.7
1	B	291	ALA	2.6
1	B	372	GLU	2.5
1	A	302	PRO	2.5
1	B	367	GLU	2.4
1	A	369	HIS	2.4
1	C	365	TYR	2.4
1	C	361	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	PRO	2.3
1	C	291	ALA	2.3
1	A	93	ARG	2.3
1	B	369	HIS	2.3
1	A	371	VAL	2.3
1	C	392	VAL	2.2
1	A	370	SER	2.2
1	B	93	ARG	2.1
1	B	366	VAL	2.1
1	C	9	ARG	2.1
1	C	307	TYR	2.1
1	C	351	GLU	2.1
1	B	392	VAL	2.1
1	B	301	SER	2.1
1	C	360	LEU	2.1
1	A	365	TYR	2.1
1	A	372	GLU	2.1
1	C	358	GLN	2.0
1	A	252	ASP	2.0
1	A	392	VAL	2.0
1	C	253	GLY	2.0
1	A	9	ARG	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.

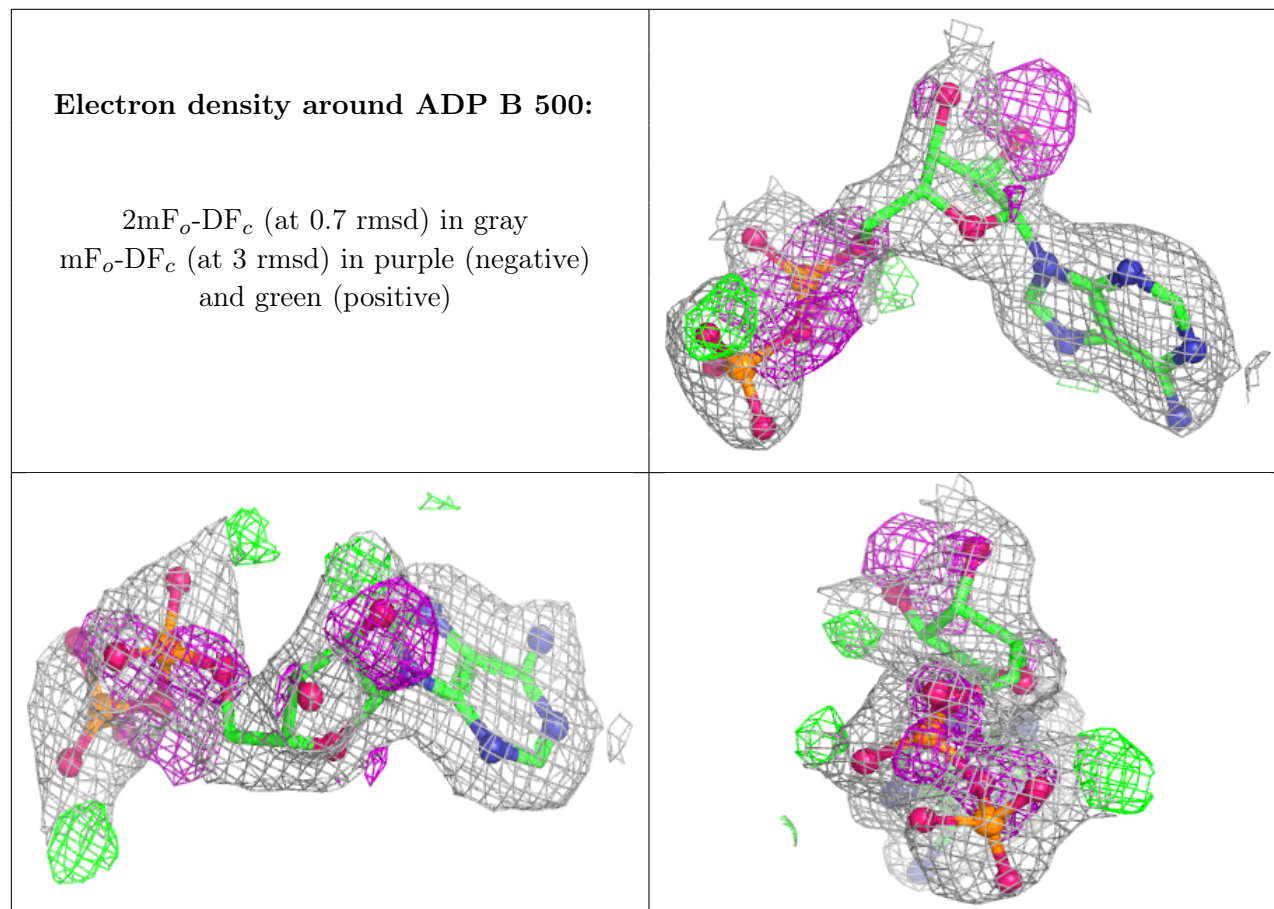
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	B	500	27/27	0.87	0.11	22,29,51,56	0

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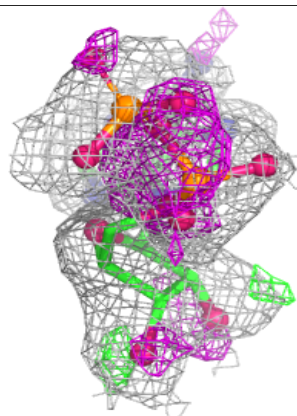
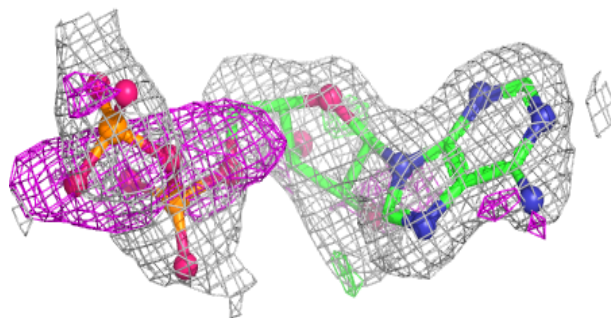
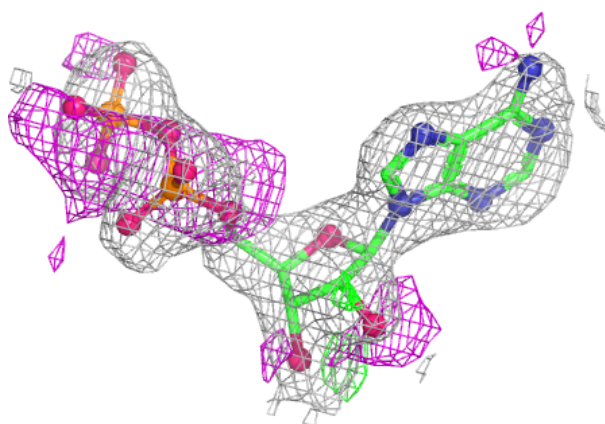
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ADP	C	500	27/27	0.87	0.11	25,33,51,53	0
2	ADP	A	500	27/27	0.90	0.10	24,35,55,57	0

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.

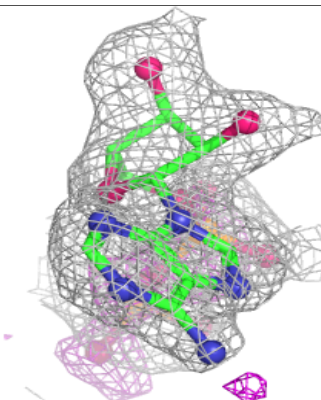
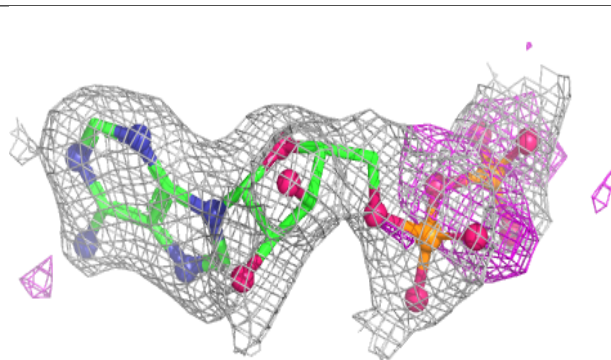
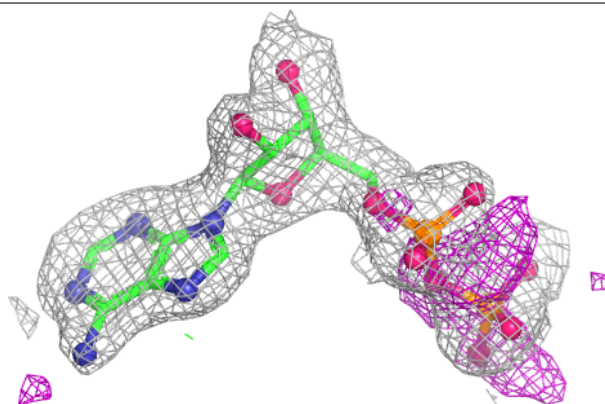


Electron density around ADP C 500:

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

**Electron density around ADP A 500:**

$2mF_o-DF_c$ (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.