



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:16 PM UTC

PDB ID : 9EB8 / pdb_00009eb8
Title : Crystal Structure of Biotin Carboxylase from Ankistrodesmus in Complex with ADP
Authors : Leonardo, D.A.C.; Vargas, J.A.S.; Mavila, A.M.; Furtado, A.A.; Pereira, H.M.; Garratt, R.C.; Castro, J.C.
Deposited on : 2024-11-12
Resolution : 1.90 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

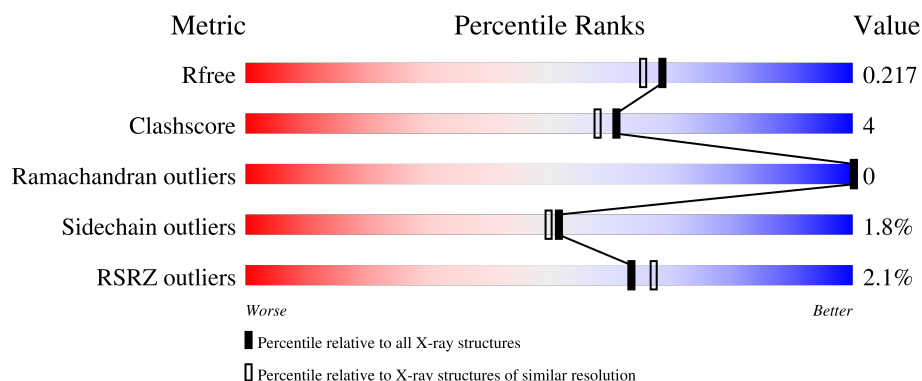
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	534	<div> <div>79%</div> <div>8%</div> <div>13%</div> </div>
1	B	534	<div> <div>4%</div> <div>78%</div> <div>9%</div> <div>13%</div> </div>
1	C	534	<div> <div>78%</div> <div>9%</div> <div>13%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	B	505	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11894 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 Biotin carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3559	2254	627	662	16			
1	B	466	Total	C	N	O	S	0	0	0
			3534	2240	620	658	16			
1	C	466	Total	C	N	O	S	0	0	0
			3547	2248	625	658	16			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-58	MET	-	expression tag	UNP A0A2U8JGP4
A	-57	GLY	-	expression tag	UNP A0A2U8JGP4
A	-56	SER	-	expression tag	UNP A0A2U8JGP4
A	-55	SER	-	expression tag	UNP A0A2U8JGP4
A	-54	HIS	-	expression tag	UNP A0A2U8JGP4
A	-53	HIS	-	expression tag	UNP A0A2U8JGP4
A	-52	HIS	-	expression tag	UNP A0A2U8JGP4
A	-51	HIS	-	expression tag	UNP A0A2U8JGP4
A	-50	HIS	-	expression tag	UNP A0A2U8JGP4
A	-49	HIS	-	expression tag	UNP A0A2U8JGP4
A	-48	SER	-	expression tag	UNP A0A2U8JGP4
A	-47	GLN	-	expression tag	UNP A0A2U8JGP4
A	-46	ASP	-	expression tag	UNP A0A2U8JGP4
A	-45	PRO	-	expression tag	UNP A0A2U8JGP4
B	-58	MET	-	expression tag	UNP A0A2U8JGP4
B	-57	GLY	-	expression tag	UNP A0A2U8JGP4
B	-56	SER	-	expression tag	UNP A0A2U8JGP4
B	-55	SER	-	expression tag	UNP A0A2U8JGP4
B	-54	HIS	-	expression tag	UNP A0A2U8JGP4
B	-53	HIS	-	expression tag	UNP A0A2U8JGP4
B	-52	HIS	-	expression tag	UNP A0A2U8JGP4
B	-51	HIS	-	expression tag	UNP A0A2U8JGP4
B	-50	HIS	-	expression tag	UNP A0A2U8JGP4

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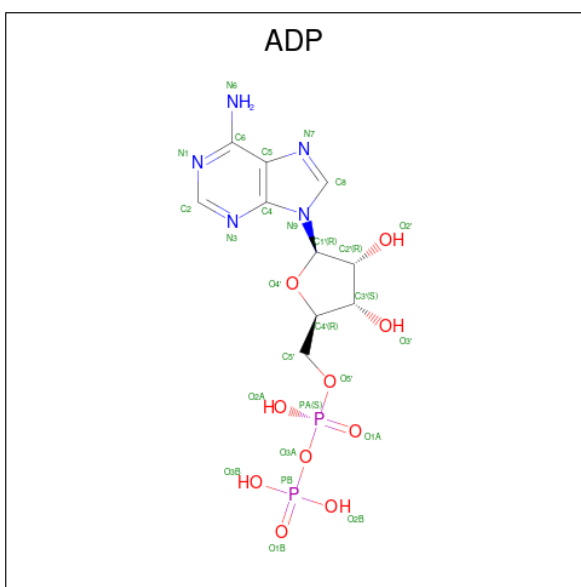
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-49	HIS	-	expression tag	UNP A0A2U8JGP4
B	-48	SER	-	expression tag	UNP A0A2U8JGP4
B	-47	GLN	-	expression tag	UNP A0A2U8JGP4
B	-46	ASP	-	expression tag	UNP A0A2U8JGP4
B	-45	PRO	-	expression tag	UNP A0A2U8JGP4
C	-58	MET	-	expression tag	UNP A0A2U8JGP4
C	-57	GLY	-	expression tag	UNP A0A2U8JGP4
C	-56	SER	-	expression tag	UNP A0A2U8JGP4
C	-55	SER	-	expression tag	UNP A0A2U8JGP4
C	-54	HIS	-	expression tag	UNP A0A2U8JGP4
C	-53	HIS	-	expression tag	UNP A0A2U8JGP4
C	-52	HIS	-	expression tag	UNP A0A2U8JGP4
C	-51	HIS	-	expression tag	UNP A0A2U8JGP4
C	-50	HIS	-	expression tag	UNP A0A2U8JGP4
C	-49	HIS	-	expression tag	UNP A0A2U8JGP4
C	-48	SER	-	expression tag	UNP A0A2U8JGP4
C	-47	GLN	-	expression tag	UNP A0A2U8JGP4
C	-46	ASP	-	expression tag	UNP A0A2U8JGP4
C	-45	PRO	-	expression tag	UNP A0A2U8JGP4

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

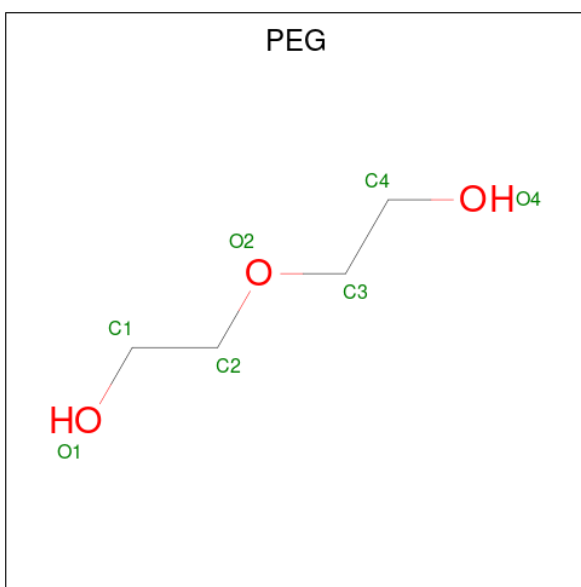
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



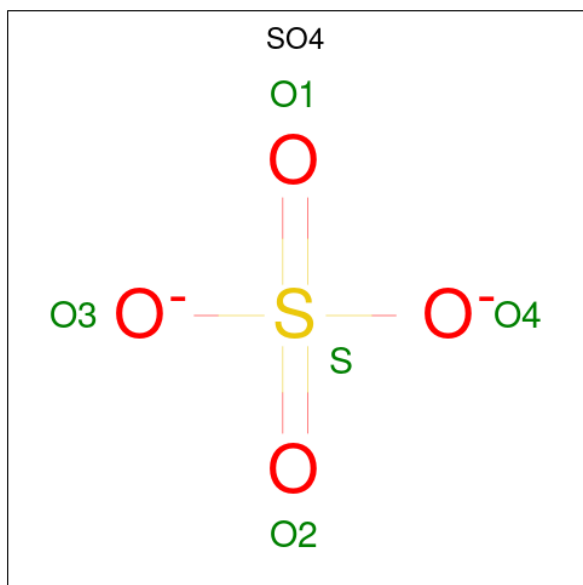
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	327	Total 327	O 327	0	0
6	B	396	Total 396	O 396	0	0
6	C	384	Total 384	O 384	0	0

E296	L307	I312	Q316	E325	K330	C336	P343	F347	R353	L371	D374	L385	E408	F420	L425	G433	T437	F459	V464	LYS	SER	GLY	LYS	SER	LYS	THR	LYS	VAL	VAL
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	177.78Å 95.36Å 95.19Å 90.00° 92.67° 90.00°	Depositor
Resolution (Å)	47.68 – 1.90 47.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.68-1.90) 99.5 (47.68-1.90)	Depositor EDS
R_{merge}	0.30	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 1.90Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.178 , 0.217 0.179 , 0.217	Depositor DCC
R_{free} test set	6333 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11894	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: PEG, ADP, MG, SO4

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	0.25	0/3635	0.46	0/4935
1	B	0.27	0/3610	0.48	0/4906
1	C	0.27	0/3623	0.49	0/4922
All	All	0.26	0/10868	0.48	0/14763

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

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	3559	0	3524	23	0
1	B	3534	0	3481	35	0
1	C	3547	0	3505	33	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
4	A	14	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	10	0	0
4	C	7	0	10	2	0
5	A	10	0	0	0	0
5	B	15	0	0	2	0
5	C	10	0	0	1	0
6	A	327	0	0	6	1
6	B	396	0	0	6	0
6	C	384	0	0	3	0
All	All	11894	0	10586	90	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 4.

All (90) 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:140:ASN:OD1	1:B:143:GLN:N	2.05	0.89
1:A:426:ASP:OD1	1:A:431:ARG:NH1	2.18	0.77
1:C:261:ASN:ND2	6:C:602:HOH:O	2.17	0.76
1:A:396:ASN:ND2	6:A:602:HOH:O	2.18	0.75
5:B:505:SO4:O3	6:B:601:HOH:O	2.10	0.69
1:C:207:ARG:NH1	6:C:604:HOH:O	2.27	0.68
5:B:505:SO4:S	6:B:601:HOH:O	2.51	0.67
1:A:207:ARG:NH1	6:A:604:HOH:O	2.23	0.67
1:A:396:ASN:ND2	6:A:606:HOH:O	2.28	0.66
1:B:408:GLU:OE1	6:B:602:HOH:O	2.14	0.64
1:C:330:LYS:HD3	4:C:503:PEG:H31	1.79	0.63
1:B:240:GLU:HG2	1:B:295:GLU:HG2	1.82	0.62
1:B:138:ILE:HG21	1:B:144:ALA:HB2	1.81	0.61
1:C:6:LEU:HB3	1:C:78:ILE:HD13	1.83	0.61
1:C:67:LEU:HD21	1:C:98:HIS:CE1	2.36	0.60
1:C:93:GLU:OE2	1:C:111:ARG:NH2	2.34	0.60
1:C:207:ARG:NH2	1:C:433:GLY:O	2.32	0.56
1:A:301:MET:HE2	1:A:389:ILE:HG22	1.89	0.55
1:B:156:MET:HE2	1:B:168:MET:HE3	1.89	0.53
1:A:353:ARG:HD3	1:A:374:ASP:OD1	2.08	0.53
1:B:177:PHE:CD2	1:B:178:LEU:HD12	2.44	0.52
1:B:105:PRO:HG3	1:B:290:THR:HB	1.92	0.52
1:B:140:ASN:HB2	1:B:142:GLN:OE1	2.08	0.52
1:B:156:MET:HE1	1:B:168:MET:HB3	1.91	0.52
1:C:111:ARG:NH1	5:C:505:SO4:O4	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:GLY:HA2	1:B:151:VAL:HG21	1.92	0.52
1:A:224:LEU:HD22	1:A:307:LEU:HD21	1.93	0.51
1:A:379:PRO:HG2	1:B:376:LEU:HD21	1.92	0.51
1:B:311:GLN:HG3	6:B:858:HOH:O	2.11	0.50
1:C:224:LEU:HD22	1:C:307:LEU:HD21	1.93	0.50
1:B:367:MET:HE3	1:B:369:SER:HB2	1.93	0.49
1:C:312:ILE:O	1:C:316:GLN:HG2	2.12	0.49
1:B:162:GLY:HA2	1:B:192:PHE:CE2	2.47	0.49
1:C:93:GLU:CD	1:C:111:ARG:HH22	2.20	0.49
1:A:201:ARG:NH1	6:A:616:HOH:O	2.42	0.48
1:C:113:MET:HA	1:C:119:ALA:HB2	1.95	0.48
1:A:82:TYR:CZ	1:A:294:VAL:HG22	2.49	0.48
1:A:162:GLY:HA2	1:A:192:PHE:CE2	2.49	0.47
1:A:427:HIS:HE2	1:A:446:GLU:CD	2.21	0.47
1:C:353:ARG:HD3	1:C:374:ASP:OD1	2.15	0.47
1:C:153:PHE:CE1	1:C:174:GLU:HB3	2.49	0.47
1:A:20:ALA:O	1:A:24:MET:HG3	2.14	0.47
1:C:336:CYS:SG	1:C:425:LEU:HD11	2.55	0.47
1:B:43:LYS:HE2	1:C:459:PHE:HB2	1.97	0.46
1:C:105:PRO:HG3	1:C:290:THR:HB	1.97	0.46
1:A:46:ASP:OD2	6:A:603:HOH:O	2.20	0.46
1:B:222:VAL:HG21	1:B:322:PHE:HE2	1.80	0.46
1:C:80:PRO:HG3	1:C:102:PHE:CZ	2.50	0.46
1:A:420:PHE:CE2	1:A:424:ILE:HD11	2.50	0.45
1:B:43:LYS:NZ	6:B:603:HOH:O	2.17	0.45
1:B:80:PRO:HB2	1:B:86:SER:HA	1.98	0.45
1:B:156:MET:CE	1:B:168:MET:HE3	2.46	0.45
1:B:222:VAL:HG21	1:B:322:PHE:CE2	2.51	0.45
1:C:80:PRO:HB2	1:C:86:SER:HA	1.98	0.45
1:C:371:LEU:HD21	1:C:385:LEU:HD22	1.97	0.45
1:A:67:LEU:HD11	1:A:94:ILE:HG22	1.98	0.45
1:C:343:PRO:HB3	1:C:347:PHE:CE1	2.51	0.45
1:A:230:SER:O	1:A:437:THR:HA	2.17	0.45
1:B:82:TYR:CZ	1:B:294:VAL:HG22	2.52	0.45
1:C:105:PRO:HG2	1:C:110:ILE:HG13	1.98	0.44
1:C:209:ILE:HD12	1:C:278:TRP:HB3	2.00	0.44
1:B:230:SER:O	1:B:437:THR:HA	2.17	0.44
1:B:410:VAL:HG21	1:B:460:LEU:HD12	1.99	0.44
1:B:404:ARG:HD2	6:C:613:HOH:O	2.17	0.44
1:A:93:GLU:OE2	1:A:111:ARG:NH2	2.51	0.44
1:B:115:ASP:HB3	1:B:118:THR:OG1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HD12	1:A:278:TRP:CB	2.48	0.44
1:C:209:ILE:HD12	1:C:278:TRP:CB	2.48	0.44
1:C:293:GLN:HG2	1:C:295:GLU:CD	2.43	0.43
1:B:343:PRO:HG3	1:B:420:PHE:HB2	2.00	0.43
1:C:105:PRO:HG2	1:C:110:ILE:CG1	2.48	0.43
1:C:230:SER:O	1:C:437:THR:HA	2.19	0.43
1:B:404:ARG:CZ	1:B:404:ARG:HB2	2.49	0.43
1:B:112:VAL:HG23	6:B:850:HOH:O	2.19	0.42
1:A:157:ILE:O	1:A:168:MET:HA	2.19	0.42
1:B:44:LEU:HD22	1:C:408:GLU:HG2	2.01	0.42
1:A:259:ALA:HA	1:A:274:ILE:HD13	2.01	0.41
1:C:233:ARG:HG2	1:C:238:LEU:HD11	2.01	0.41
1:A:393:GLU:HG3	6:A:814:HOH:O	2.20	0.41
1:C:233:ARG:NH1	1:C:236:GLN:OE1	2.53	0.41
1:B:162:GLY:HA2	1:B:192:PHE:CZ	2.55	0.41
1:A:67:LEU:HD11	1:A:94:ILE:CG2	2.51	0.41
1:B:420:PHE:CE2	1:B:424:ILE:HD11	2.55	0.41
1:B:113:MET:HA	1:B:119:ALA:HB2	2.03	0.41
1:B:343:PRO:CG	1:B:420:PHE:HB2	2.51	0.41
1:C:330:LYS:HB3	4:C:503:PEG:H22	2.03	0.40
1:B:209:ILE:HD12	1:B:278:TRP:CB	2.51	0.40
1:C:178:LEU:HD23	1:C:178:LEU:HA	1.83	0.40
1:B:295:GLU:H	1:B:295:GLU:CD	2.29	0.40
1:C:343:PRO:CG	1:C:420:PHE:HB2	2.50	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:619:HOH:O	6:A:619:HOH:O[2_556]	2.02	0.18

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	464/534 (87%)	455 (98%)	9 (2%)	0	100	100
1	B	464/534 (87%)	457 (98%)	7 (2%)	0	100	100
1	C	464/534 (87%)	456 (98%)	8 (2%)	0	100	100
All	All	1392/1602 (87%)	1368 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/429 (86%)	361 (98%)	8 (2%)	45	42
1	B	364/429 (85%)	358 (98%)	6 (2%)	55	54
1	C	366/429 (85%)	360 (98%)	6 (2%)	55	54
All	All	1099/1287 (85%)	1079 (98%)	20 (2%)	51	50

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	40	LEU
1	A	78	ILE
1	A	118	THR
1	A	142	GLN
1	A	180	LEU
1	A	247	LEU
1	A	301	MET
1	B	26	LEU
1	B	78	ILE
1	B	247	LEU
1	B	253	GLN
1	B	295	GLU
1	B	410	VAL

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Mol	Chain	Res	Type
1	C	26	LEU
1	C	44	LEU
1	C	247	LEU
1	C	293	GLN
1	C	316	GLN
1	C	325	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN
1	A	396	ASN
1	B	232	GLN
1	B	318	HIS
1	C	205	ASN
1	C	235	ASN
1	C	309	GLN
1	C	318	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 17 ligands modelled in this entry, 3 are monoatomic - leaving 14 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	PEG	C	503	-	6,6,6	0.12	0	5,5,5	0.12	0
5	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.07	0
4	PEG	A	504	-	6,6,6	0.11	0	5,5,5	0.12	0
4	PEG	A	503	-	6,6,6	0.14	0	5,5,5	0.08	0
5	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.16	0
5	SO4	B	505	-	4,4,4	0.30	0	6,6,6	0.12	0
3	ADP	C	502	2	28,29,29	1.39	3 (10%)	43,45,45	1.84	8 (18%)
3	ADP	A	502	2	28,29,29	1.39	4 (14%)	43,45,45	1.73	8 (18%)
5	SO4	B	506	-	4,4,4	0.24	0	6,6,6	0.16	0
3	ADP	B	502	2	28,29,29	1.40	5 (17%)	43,45,45	1.70	9 (20%)
4	PEG	B	503	-	6,6,6	0.12	0	5,5,5	0.10	0
5	SO4	A	506	-	4,4,4	0.27	0	6,6,6	0.17	0
5	SO4	B	504	-	4,4,4	0.24	0	6,6,6	0.14	0
5	SO4	A	505	-	4,4,4	0.29	0	6,6,6	0.19	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	PEG	C	503	-	-	2/4/4/4	-
4	PEG	A	504	-	-	2/4/4/4	-
4	PEG	A	503	-	-	2/4/4/4	-
3	ADP	C	502	2	-	1/16/32/32	0/3/3/3
3	ADP	A	502	2	-	2/16/32/32	0/3/3/3
3	ADP	B	502	2	-	1/16/32/32	0/3/3/3
4	PEG	B	503	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	ADP	C5-C4	4.76	1.47	1.39
3	A	502	ADP	C5-C4	4.74	1.47	1.39
3	C	502	ADP	C5-C4	4.70	1.47	1.39
3	C	502	ADP	C5-C6	2.82	1.48	1.41
3	B	502	ADP	C5-C6	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	ADP	C5-C6	2.49	1.47	1.41
3	A	502	ADP	C5-N7	-2.45	1.34	1.39
3	C	502	ADP	C8-N7	2.30	1.36	1.31
3	B	502	ADP	C8-N7	2.23	1.36	1.31
3	B	502	ADP	C4-N9	-2.20	1.33	1.37
3	B	502	ADP	C5-N7	-2.20	1.35	1.39
3	A	502	ADP	C8-N7	2.14	1.35	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ADP	C5-C4-N3	-5.87	118.63	126.72
3	A	502	ADP	C5-C4-N3	-5.36	119.33	126.72
3	B	502	ADP	C5-C4-N3	-4.99	119.84	126.72
3	C	502	ADP	N3-C4-N9	4.75	135.24	127.17
3	A	502	ADP	N3-C4-N9	4.51	134.84	127.17
3	B	502	ADP	N3-C4-N9	4.13	134.19	127.17
3	C	502	ADP	C2-N3-C4	3.81	121.14	111.83
3	A	502	ADP	C2-N3-C4	3.50	120.37	111.83
3	B	502	ADP	N3-C2-N1	-3.47	123.33	128.58
3	C	502	ADP	N3-C2-N1	-3.43	123.39	128.58
3	A	502	ADP	N3-C2-N1	-3.42	123.41	128.58
3	B	502	ADP	C2-N3-C4	3.36	120.03	111.83
3	C	502	ADP	C4-C5-N7	-3.24	106.88	110.58
3	B	502	ADP	C4-C5-N7	-3.02	107.13	110.58
3	B	502	ADP	C4-N9-C8	2.85	108.73	105.74
3	A	502	ADP	C4-C5-N7	-2.79	107.39	110.58
3	C	502	ADP	C4-N9-C8	2.58	108.44	105.74
3	A	502	ADP	C4-N9-C8	2.54	108.40	105.74
3	B	502	ADP	C2-N1-C6	2.42	122.70	118.73
3	C	502	ADP	O2A-PA-O3A	2.40	113.77	107.27
3	C	502	ADP	C5-N7-C8	2.37	107.17	103.45
3	A	502	ADP	C2-N1-C6	2.28	122.47	118.73
3	B	502	ADP	C6-C5-N7	2.17	136.27	132.09
3	B	502	ADP	C5-N7-C8	2.11	106.77	103.45
3	A	502	ADP	C5-N7-C8	2.08	106.72	103.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	PEG	O2-C3-C4-O4

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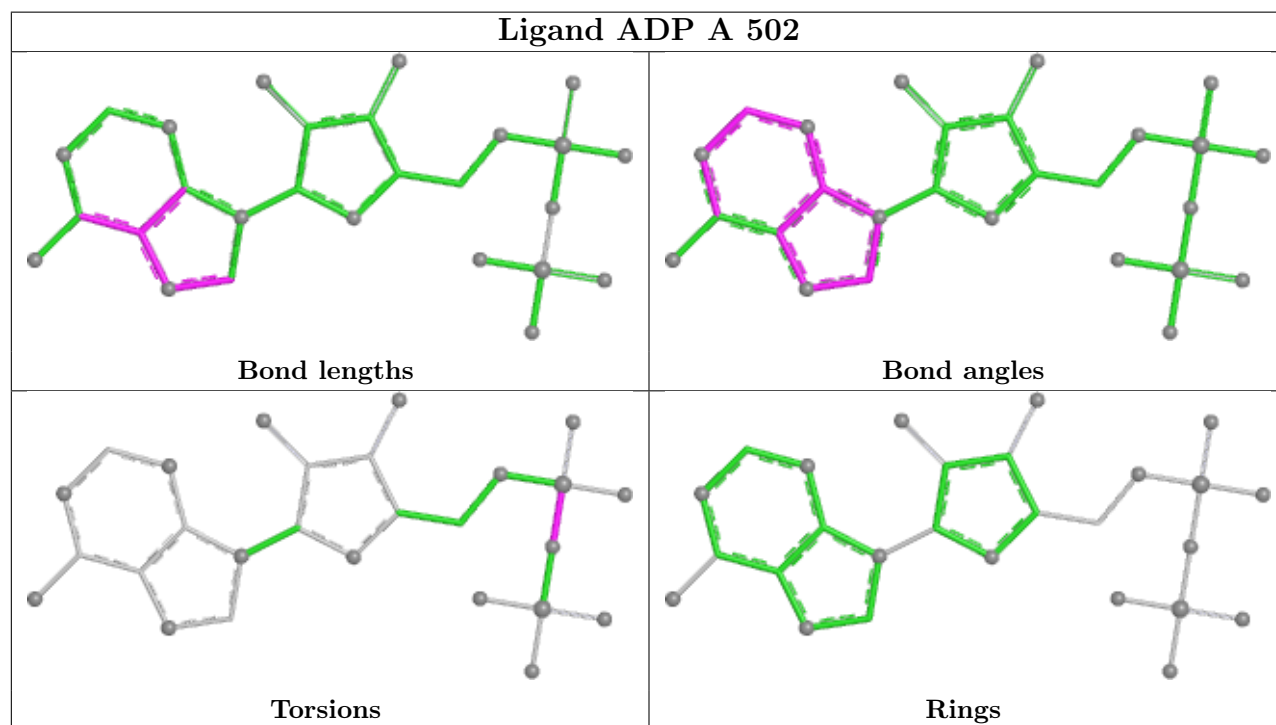
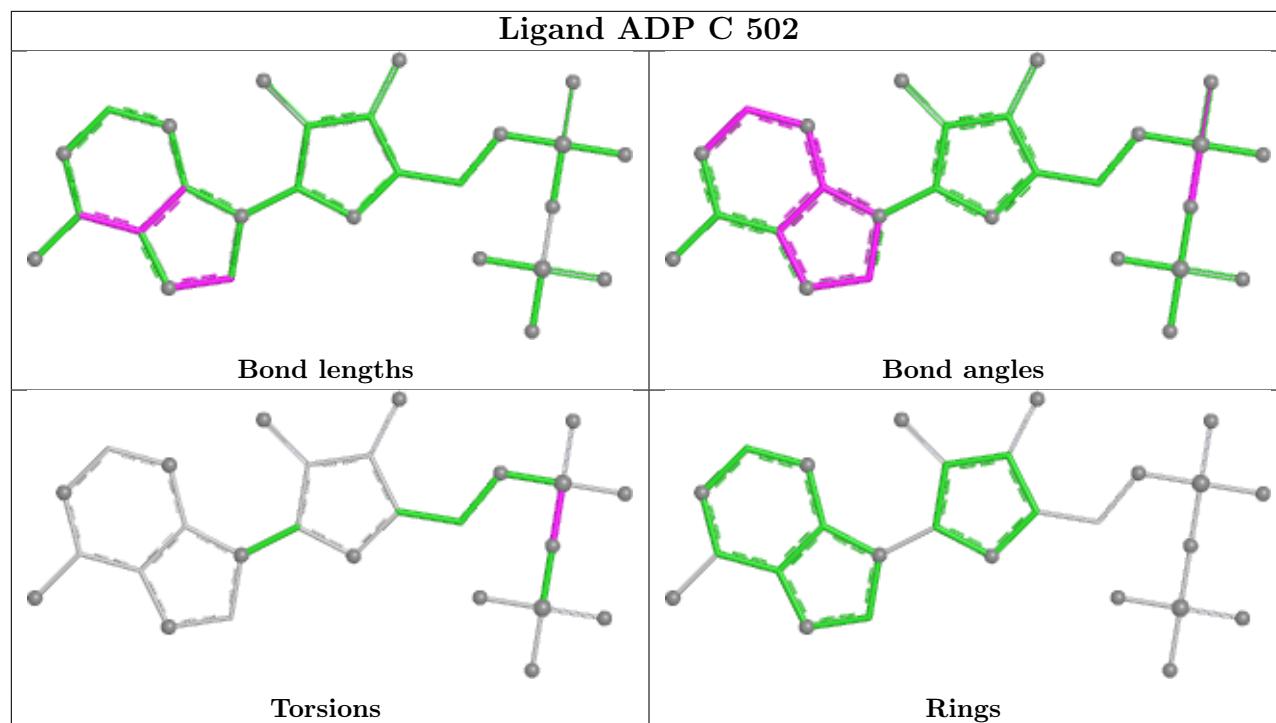
Mol	Chain	Res	Type	Atoms
4	C	503	PEG	O2-C3-C4-O4
4	A	504	PEG	O1-C1-C2-O2
4	C	503	PEG	O1-C1-C2-O2
4	A	503	PEG	O1-C1-C2-O2
4	B	503	PEG	C1-C2-O2-C3
4	A	504	PEG	C4-C3-O2-C2
3	C	502	ADP	PB-O3A-PA-O1A
4	A	503	PEG	C4-C3-O2-C2
3	A	502	ADP	PB-O3A-PA-O1A
3	A	502	ADP	PB-O3A-PA-O2A
3	B	502	ADP	PB-O3A-PA-O1A

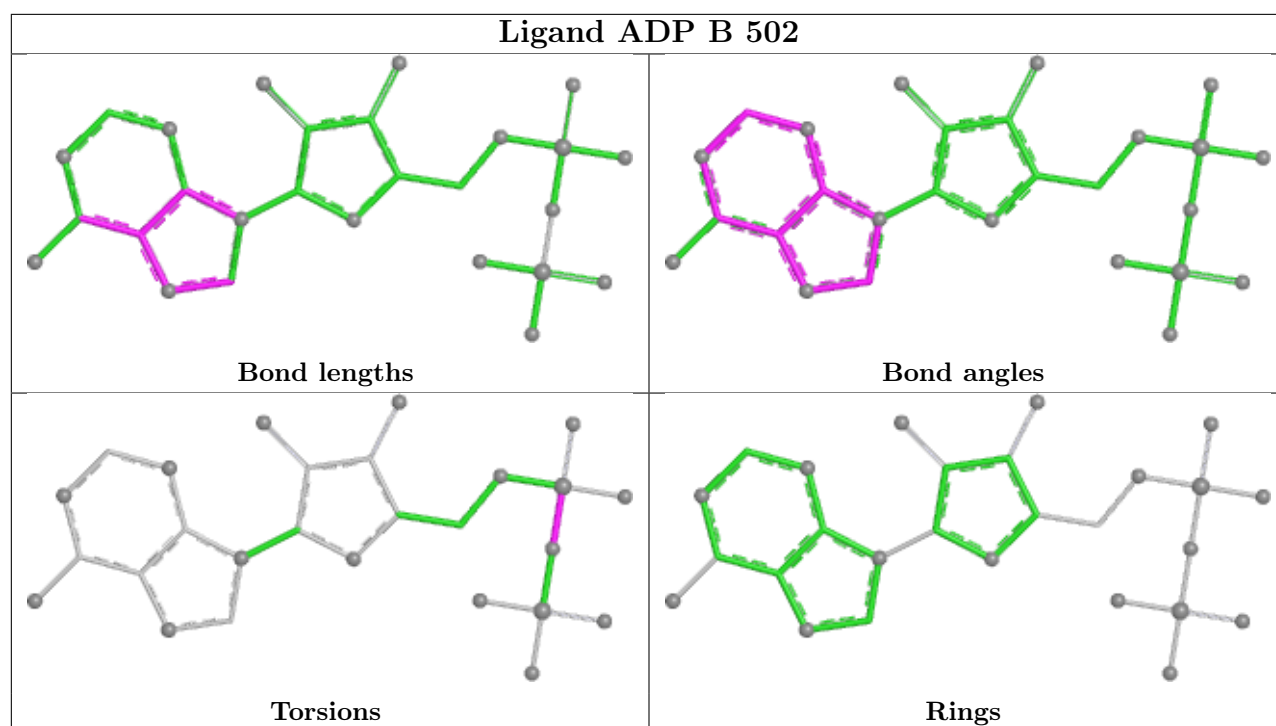
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	503	PEG	2	0
5	C	505	SO4	1	0
5	B	505	SO4	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	466/534 (87%)	0.05	8 (1%) 69 72	14, 25, 40, 59	0
1	B	466/534 (87%)	0.09	20 (4%) 40 42	15, 24, 41, 67	0
1	C	466/534 (87%)	0.00	2 (0%) 88 90	15, 24, 37, 49	0
All	All	1398/1602 (87%)	0.05	30 (2%) 63 67	14, 25, 39, 67	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	141	ASP	3.9
1	B	137	LEU	3.6
1	A	466	SER	3.4
1	A	124	LYS	3.3
1	A	121	ASP	3.3
1	C	139	GLU	3.2
1	A	465	LYS	2.9
1	B	1	ASP	2.9
1	B	434	ASP	2.8
1	B	149	ASN	2.8
1	A	125	LYS	2.6
1	B	138	ILE	2.6
1	B	163	GLY	2.5
1	B	322	PHE	2.5
1	B	466	SER	2.4
1	C	67	LEU	2.4
1	B	150	GLN	2.3
1	A	53	ASP	2.3
1	B	175	GLU	2.3
1	B	151	VAL	2.2
1	A	174	GLU	2.2
1	B	407	ASP	2.2
1	B	179	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	140	ASN	2.1
1	B	176	GLU	2.1
1	B	382	ASP	2.1
1	B	162	GLY	2.0
1	B	178	LEU	2.0
1	A	407	ASP	2.0
1	B	444	GLN	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.

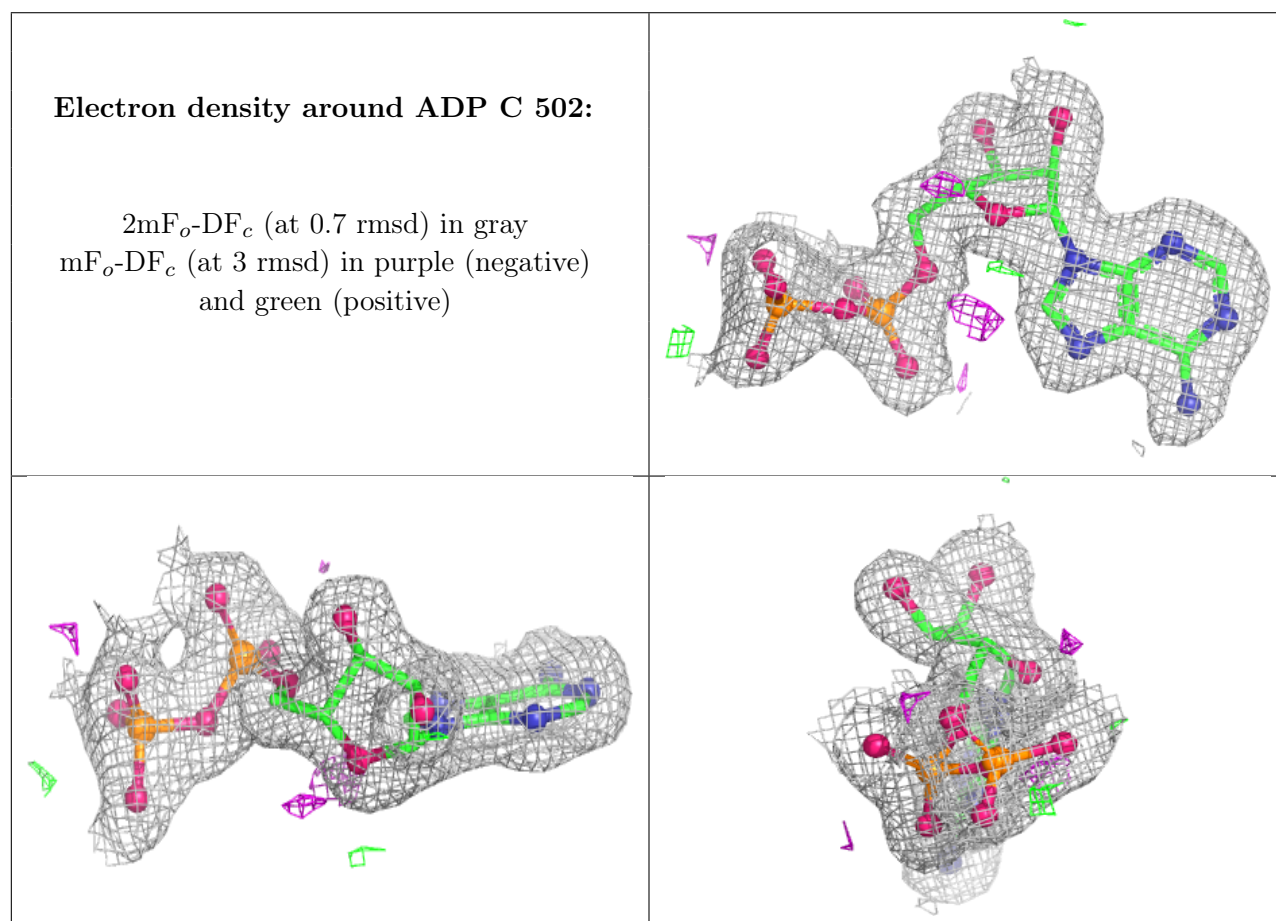
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	B	506	5/5	0.67	0.14	44,45,62,81	0
5	SO4	C	505	5/5	0.84	0.09	52,64,66,89	0
4	PEG	A	504	7/7	0.85	0.13	24,31,41,46	0
5	SO4	B	505	5/5	0.85	0.11	36,39,53,56	0
4	PEG	C	503	7/7	0.87	0.12	24,36,41,42	0
4	PEG	A	503	7/7	0.88	0.11	28,31,33,42	0
4	PEG	B	503	7/7	0.91	0.09	29,33,38,39	0
5	SO4	A	506	5/5	0.92	0.09	45,48,51,52	0
5	SO4	C	504	5/5	0.93	0.10	37,37,39,43	0
5	SO4	A	505	5/5	0.95	0.10	30,38,44,44	0
5	SO4	B	504	5/5	0.96	0.10	39,40,42,43	0
3	ADP	C	502	27/27	0.98	0.05	18,20,26,26	0
3	ADP	A	502	27/27	0.98	0.05	16,21,25,28	0
3	ADP	B	502	27/27	0.98	0.05	18,22,28,34	0
2	MG	C	501	1/1	0.99	0.03	22,22,22,22	0
2	MG	A	501	1/1	0.99	0.03	21,21,21,21	0

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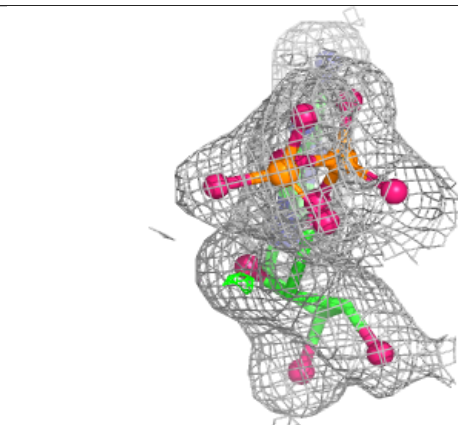
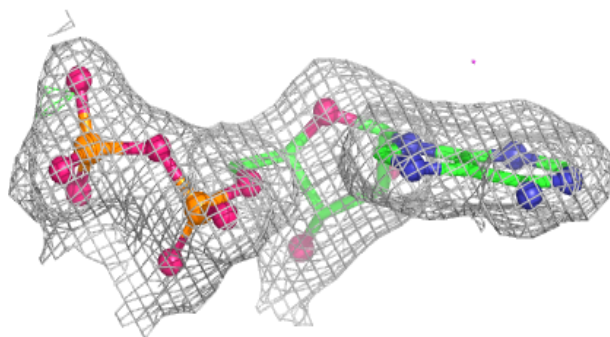
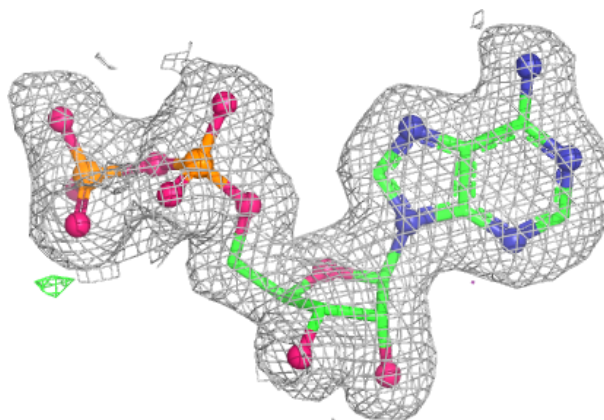
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	B	501	1/1	0.99	0.03	20,20,20,20	0

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.

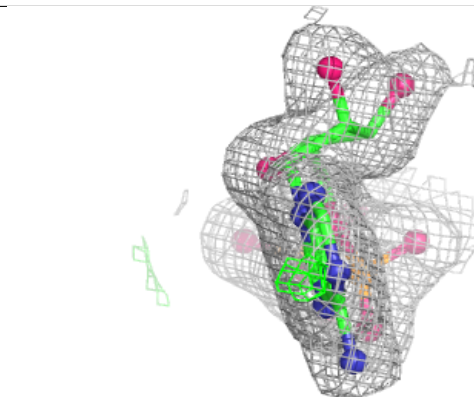
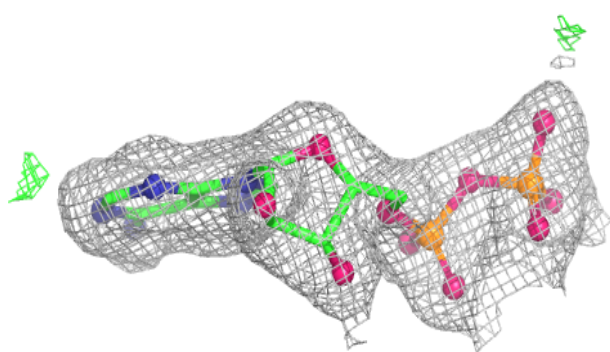
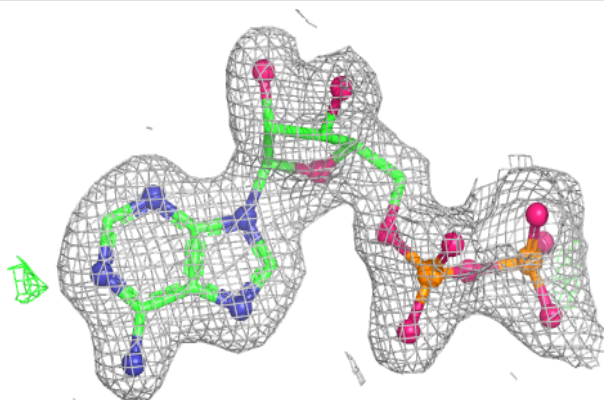


Electron density around ADP A 502:

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

**Electron density around ADP 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.