



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 09:45 AM EDT

PDB ID : 4RVO  
Title : Crystal structure of a Putative Acyl-CoA ligase (BT\_0428) from Bacteroides  
thetaiotaomicron VPI-5482 at 2.41 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2014-11-26  
Resolution : 2.41 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](mailto: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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

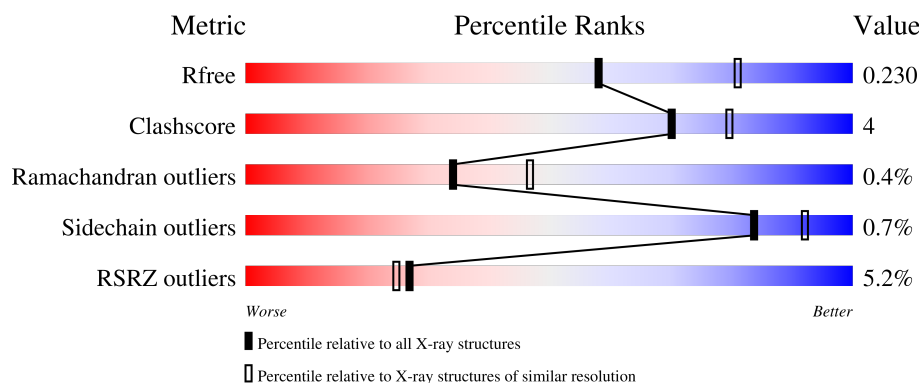
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.41 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))
$R_{free}$	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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  $\geq 3$ , 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	436	 3% 92% 7%
1	B	436	 8% 91% 7% .
1	C	436	 3% 93% 7%
1	D	436	 6% 89% 9% .

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	UNL	A	506	-	-	X	-
5	UNL	B	503	-	-	X	-
5	UNL	C	505	-	-	X	-
5	UNL	D	504	-	-	X	-

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 14424 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 Phenylacetate-coenzyme A ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	Se	0	6	0
			3444	2170	598	655	6	15			
1	B	428	Total	C	N	O	S	Se	0	4	0
			3353	2115	580	638	6	14			
1	C	434	Total	C	N	O	S	Se	0	4	0
			3426	2160	595	649	6	16			
1	D	428	Total	C	N	O	S	Se	0	5	0
			3363	2123	583	637	6	14			

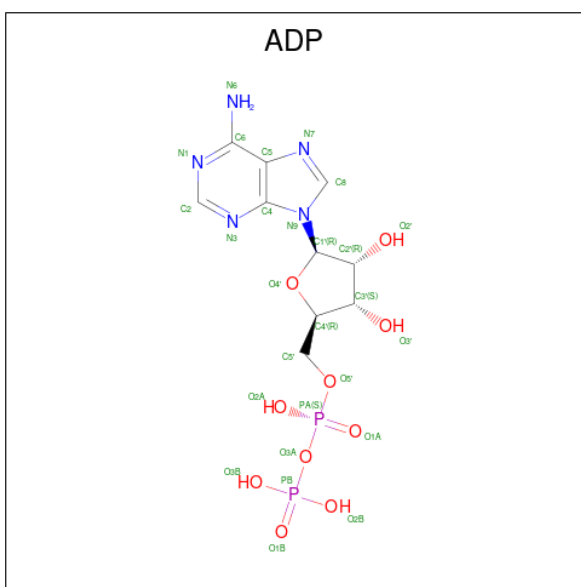
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q8AAN6
B	0	GLY	-	EXPRESSION TAG	UNP Q8AAN6
C	0	GLY	-	EXPRESSION TAG	UNP Q8AAN6
D	0	GLY	-	EXPRESSION TAG	UNP Q8AAN6

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	K	0	0
			3	3		
4	C	2	Total	K	0	0
			2	2		
4	D	1	Total	K	0	0
			1	1		

- Molecule 5 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

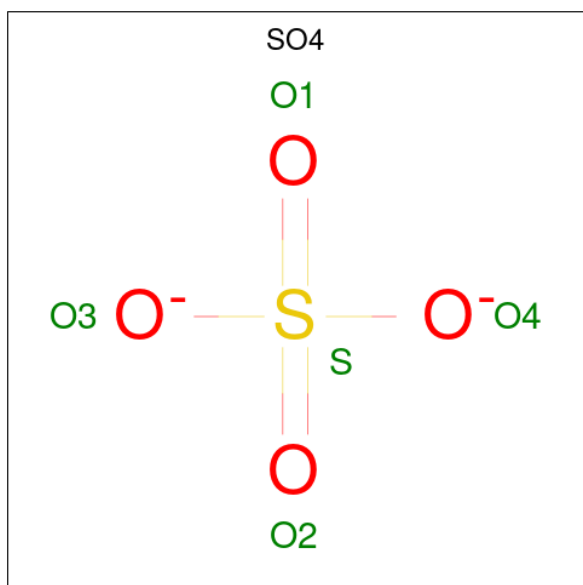
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			7	7		
5	B	1	Total	O	0	0
			8	8		

*Continued on next page...*

Continued from previous page...

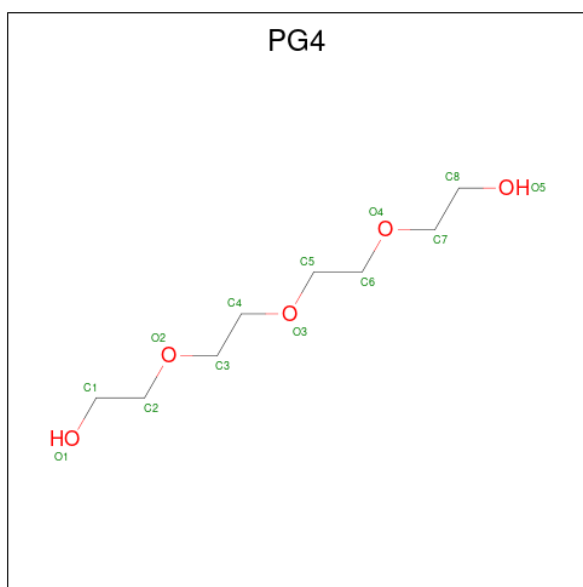
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O 13 13	0	0
5	D	1	Total O 9 9	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



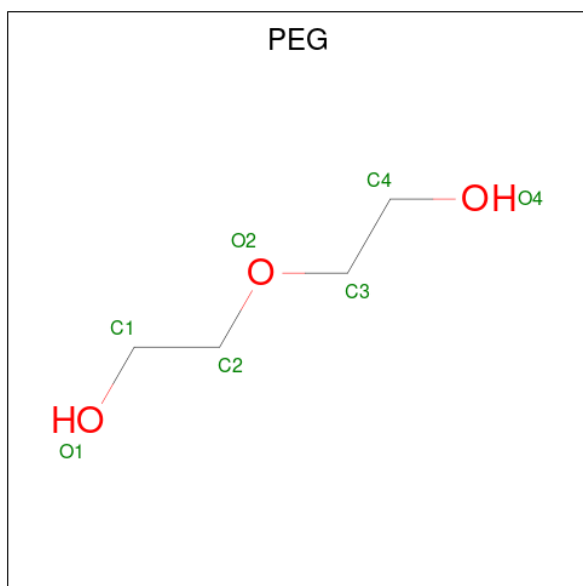
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0

- Molecule 7 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



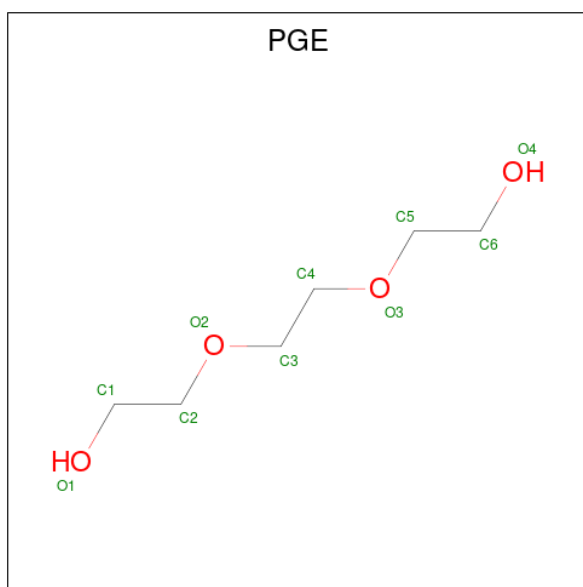
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



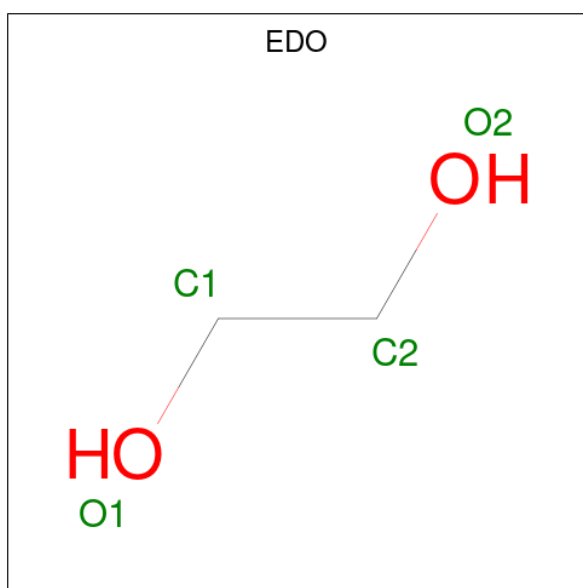
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			7	4	3		
8	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		
9	C	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		
10	A	1	Total	C	O	0	0
			4	2	2		

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	A	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	B	1	Total C O 4 2 2	0	0
10	C	1	Total C O 4 2 2	0	0
10	C	1	Total C O 4 2 2	0	0
10	C	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0
10	D	1	Total C O 4 2 2	0	0

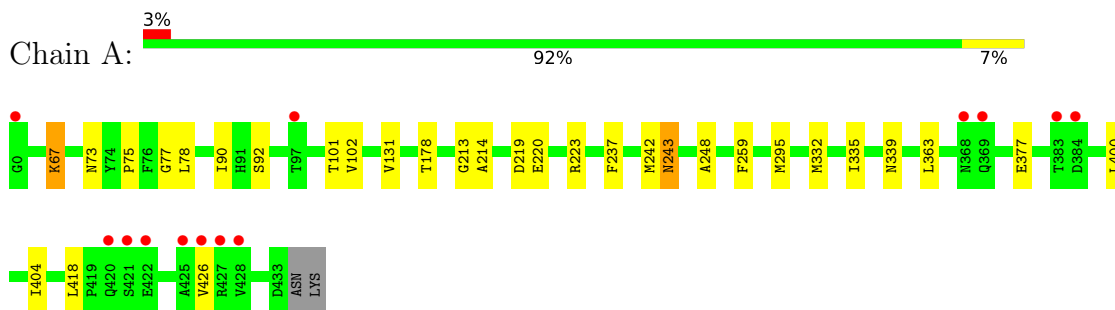
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	161	Total O 161 161	0	0
11	B	131	Total O 133 133	0	2
11	C	120	Total O 120 120	0	0
11	D	131	Total O 131 131	0	2

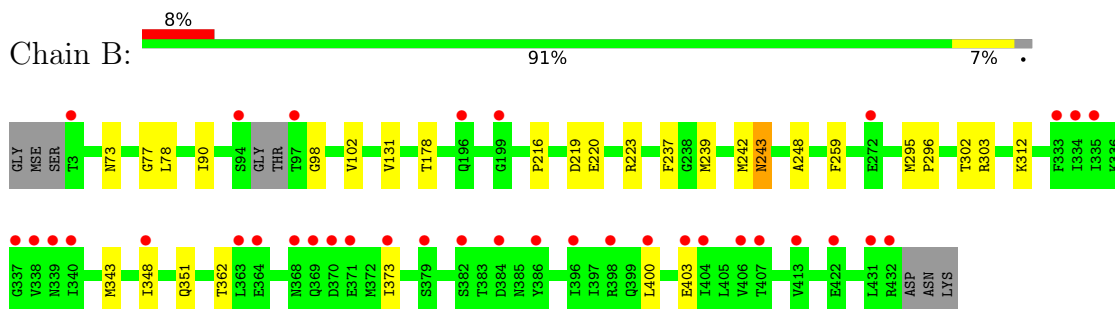
### 3 Residue-property plots

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

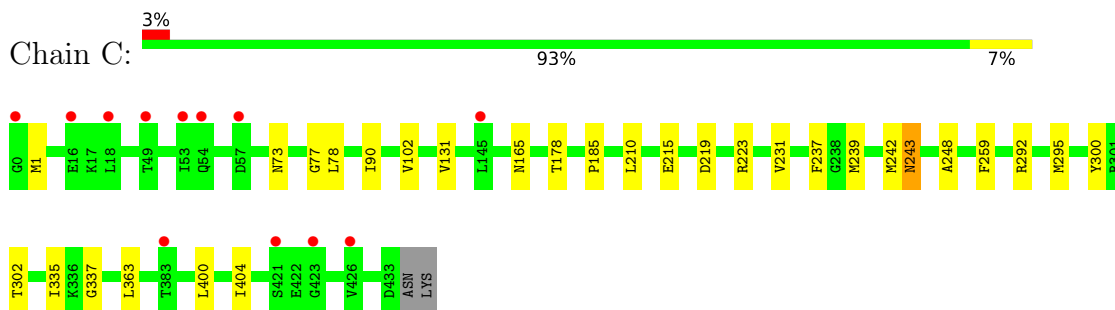
#### • Molecule 1: Phenylacetate-coenzyme A ligase



#### • Molecule 1: Phenylacetate-coenzyme A ligase

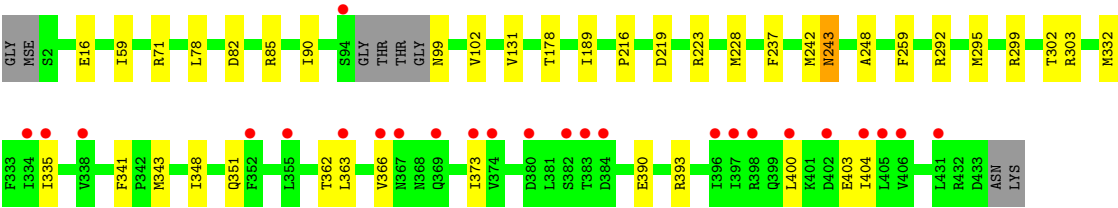


#### • Molecule 1: Phenylacetate-coenzyme A ligase



#### • Molecule 1: Phenylacetate-coenzyme A ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.24Å 210.22Å 71.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.57 – 2.41 46.57 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.57-2.41) 98.8 (46.57-2.41)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.42Å)	Xtriage
Refinement program	BUSTER-TNT 2.10.0, BUSTER 2.10.0	Depositor
R, $R_{free}$	0.187 , 0.214 0.206 , 0.230	Depositor DCC
$R_{free}$ test set	3726 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 55.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	14424	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, ADP, PG4, UNL, PEG, PGE, SO4, ZN, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/3503	0.22	0/4707
1	B	0.51	0/3409	0.22	0/4585
1	C	0.51	0/3482	0.22	0/4681
1	D	0.52	0/3421	0.22	0/4601
All	All	0.51	0/13815	0.22	0/18574

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	3444	0	3426	16	0
1	B	3353	0	3281	22	0
1	C	3426	0	3401	18	0
1	D	3363	0	3304	24	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
4	A	3	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
5	A	7	0	0	4	0
5	B	8	0	0	2	0
5	C	13	0	0	7	0
5	D	9	0	0	7	0
6	A	15	0	0	0	0
6	B	10	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
7	A	13	0	18	0	0
8	A	7	0	10	0	0
8	B	7	0	10	0	0
9	A	10	0	14	0	0
9	C	10	0	14	0	0
10	A	20	0	30	0	0
10	B	12	0	18	0	0
10	C	12	0	18	0	0
10	D	12	0	18	0	0
11	A	161	0	0	1	0
11	B	133	0	0	1	0
11	C	120	0	0	0	0
11	D	131	0	0	0	0
All	All	14424	0	13610	100	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 4.

All (100) 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)
5:C:505:UNL:O11	5:C:505:UNL:O10	1.86	0.93
5:C:505:UNL:O3	5:C:505:UNL:O4	1.86	0.92
5:B:503:UNL:O3	5:B:503:UNL:O4	1.88	0.90
3:A:502:ADP:O2B	5:A:506:UNL:O1	1.93	0.86
1:B:239:MSE:HE1	1:B:302:THR:HG22	1.57	0.85
1:D:216:PRO:HB2	1:D:343:MSE:HE3	1.61	0.82

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:501:ADP:O3B	5:D:504:UNL:O1	2.01	0.78
1:B:216:PRO:HB2	1:B:343:MSE:HE3	1.65	0.77
5:C:505:UNL:O3	5:C:505:UNL:O2	2.02	0.76
1:A:67:LYS:HA	1:A:67:LYS:HE2	1.69	0.74
1:D:71:ARG:HD3	1:D:99:ASN:HB2	1.73	0.69
5:A:506:UNL:O2	5:A:506:UNL:O3	2.10	0.69
5:C:505:UNL:O5	5:C:505:UNL:O6	2.12	0.68
5:D:504:UNL:O5	5:D:504:UNL:O6	2.11	0.67
5:D:504:UNL:O2	5:D:504:UNL:O3	2.11	0.67
5:B:503:UNL:O4	5:B:503:UNL:O5	2.14	0.66
5:C:505:UNL:O7	5:C:505:UNL:O8	2.13	0.65
1:C:237:PHE:HB3	1:C:248:ALA:HB3	1.82	0.61
5:A:506:UNL:O1	5:A:506:UNL:O2	2.19	0.60
1:B:348:ILE:O	1:B:351:GLN:HG2	2.03	0.59
3:C:502:ADP:O2B	5:C:505:UNL:O1	2.20	0.59
1:B:239:MSE:HE2	1:B:242:MSE:HG2	1.85	0.59
1:B:239:MSE:HE2	1:B:242:MSE:CG	2.33	0.58
5:A:506:UNL:O6	5:A:506:UNL:O7	2.21	0.57
5:D:504:UNL:O1	5:D:504:UNL:O4	2.22	0.57
1:A:73:ASN:HB3	1:A:77:GLY:HA3	1.87	0.56
1:D:242:MSE:O	1:D:243:ASN:HB2	2.06	0.56
1:D:335:ILE:HD13	1:D:363:LEU:HD22	1.88	0.55
1:D:78:LEU:HB2	1:D:295:MSE:HE3	1.88	0.55
1:D:90:ILE:HG23	1:D:102:VAL:HG13	1.87	0.55
1:A:237:PHE:HB3	1:A:248:ALA:HB3	1.88	0.54
1:D:362:THR:HB	1:D:373:ILE:CG2	2.37	0.54
1:B:242:MSE:O	1:B:243:ASN:HB2	2.07	0.54
1:C:73:ASN:HB3	1:C:77:GLY:HA3	1.89	0.54
1:C:335:ILE:HD13	1:C:363:LEU:HD22	1.90	0.54
1:D:348:ILE:HD12	1:D:400:LEU:HD23	1.90	0.54
1:D:348:ILE:HD11	1:D:403:GLU:CB	2.38	0.53
1:B:362:THR:HB	1:B:373:ILE:CG2	2.38	0.53
1:A:335:ILE:HD13	1:A:363:LEU:HD22	1.91	0.53
1:B:73:ASN:HB3	1:B:77:GLY:HA3	1.90	0.53
1:C:78:LEU:HB2	1:C:295:MSE:HE3	1.90	0.52
1:B:237:PHE:HB3	1:B:248:ALA:HB3	1.92	0.52
1:D:237:PHE:HB3	1:D:248:ALA:HB3	1.92	0.52
1:A:78:LEU:HB2	1:A:295:MSE:HE3	1.91	0.51
1:A:219:ASP:O	1:A:223:ARG:HG2	2.11	0.51
1:A:332:MSE:SE	1:A:339:ASN:HB3	2.61	0.51
1:C:1:MSE:HA	1:C:1:MSE:HE3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:PRO:HD2	1:C:215[A]:GLU:HG2	1.93	0.50
1:C:242:MSE:O	1:C:243:ASN:HB2	2.11	0.50
1:D:242:MSE:O	1:D:243:ASN:CB	2.59	0.50
1:D:332:MSE:HE3	1:D:341:PHE:CE2	2.46	0.50
1:D:390:GLU:OE2	1:D:393:ARG:NH1	2.44	0.50
1:C:400:LEU:O	1:C:404:ILE:HG12	2.12	0.49
1:D:400:LEU:O	1:D:404:ILE:HG12	2.12	0.49
1:B:239:MSE:CE	1:B:242:MSE:HG2	2.42	0.49
1:A:400:LEU:O	1:A:404:ILE:HG12	2.12	0.49
1:A:75:PRO:HD2	11:A:626:HOH:O	2.11	0.48
1:C:239:MSE:CE	1:C:300:TYR:HE2	2.25	0.48
5:C:505:UNL:O6	5:C:505:UNL:O7	2.32	0.48
1:B:348:ILE:HD12	1:B:400:LEU:HD23	1.96	0.48
1:C:215[B]:GLU:HG3	1:C:337:GLY:HA2	1.95	0.48
1:B:90:ILE:HG23	1:B:102:VAL:HG13	1.95	0.47
1:B:78:LEU:HB2	1:B:295:MSE:HE3	1.96	0.47
1:B:219:ASP:O	1:B:223:ARG:HG2	2.15	0.47
1:D:348:ILE:HD11	1:D:403:GLU:HB2	1.97	0.46
1:C:219:ASP:O	1:C:223:ARG:HG2	2.14	0.46
1:D:219:ASP:O	1:D:223:ARG:HG2	2.15	0.46
1:D:189:ILE:HG23	1:D:228:MSE:HE1	1.98	0.46
1:D:362:THR:HB	1:D:373:ILE:HG23	1.98	0.46
1:A:242:MSE:O	1:A:243:ASN:HB2	2.15	0.46
1:C:90:ILE:HG23	1:C:102:VAL:HG13	1.97	0.45
5:D:504:UNL:O6	5:D:504:UNL:O7	2.35	0.45
1:B:302:THR:O	1:B:303:ARG:HB2	2.17	0.45
1:D:131:VAL:HB	1:D:178:THR:HA	1.99	0.45
1:B:362:THR:HB	1:B:373:ILE:HG23	1.99	0.45
1:C:210:LEU:HD13	1:C:231:VAL:HG21	1.99	0.45
1:D:59:ILE:O	1:D:299:ARG:HD2	2.17	0.44
1:C:243:ASN:OD1	1:C:292:ARG:HD3	2.17	0.44
1:A:90:ILE:HG23	1:A:102:VAL:HG13	1.98	0.44
1:B:131:VAL:HB	1:B:178:THR:HA	2.00	0.44
1:A:242:MSE:O	1:A:243:ASN:CB	2.66	0.44
1:A:131:VAL:HB	1:A:178:THR:HA	2.01	0.43
1:C:131:VAL:HB	1:C:178:THR:HA	1.99	0.43
1:C:239:MSE:HE1	1:C:300:TYR:HE2	1.83	0.43
5:D:504:UNL:O5	5:D:504:UNL:O7	2.37	0.43
1:B:242:MSE:O	1:B:243:ASN:CB	2.67	0.43
5:D:504:UNL:O1	5:D:504:UNL:O3	2.37	0.42
1:A:92:SER:HA	1:A:101:THR:O	2.19	0.42

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HD2	11:B:617:HOH:O	2.18	0.42
1:C:239:MSE:HE1	1:C:302:THR:HA	2.01	0.42
1:D:243:ASN:OD1	1:D:292:ARG:HD3	2.20	0.42
1:C:242:MSE:O	1:C:243:ASN:CB	2.67	0.41
1:D:216:PRO:HB2	1:D:343:MSE:CE	2.40	0.41
1:D:302:THR:O	1:D:303:ARG:HB2	2.21	0.41
1:A:377[A]:GLU:HG3	1:A:418:LEU:HD12	2.02	0.41
1:B:312:LYS:NZ	1:B:312:LYS:HB3	2.35	0.41
1:D:82:ASP:CG	1:D:85:ARG:HG2	2.41	0.41
1:B:348:ILE:HD11	1:B:403:GLU:CB	2.51	0.40
1:A:213:GLY:O	1:A:214:ALA:HB3	2.21	0.40
1:B:239:MSE:HE2	1:B:242:MSE:HG3	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	438/436 (100%)	422 (96%)	14 (3%)	2 (0%)	29	40
1	B	428/436 (98%)	412 (96%)	14 (3%)	2 (0%)	29	40
1	C	436/436 (100%)	417 (96%)	18 (4%)	1 (0%)	47	61
1	D	429/436 (98%)	410 (96%)	17 (4%)	2 (0%)	29	40
All	All	1731/1744 (99%)	1661 (96%)	63 (4%)	7 (0%)	34	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	243	ASN
1	C	243	ASN
1	D	243	ASN

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	243	ASN
1	D	366	VAL
1	A	426	VAL
1	B	98	GLY

### 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	374/370 (101%)	371 (99%)	3 (1%)	81	91
1	B	356/370 (96%)	353 (99%)	3 (1%)	81	91
1	C	370/370 (100%)	368 (100%)	2 (0%)	88	95
1	D	359/370 (97%)	356 (99%)	3 (1%)	81	91
All	All	1459/1480 (99%)	1448 (99%)	11 (1%)	84	91

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	LYS
1	A	220	GLU
1	A	259	PHE
1	B	220[A]	GLU
1	B	220[B]	GLU
1	B	259	PHE
1	C	165	ASN
1	C	259	PHE
1	D	16	GLU
1	D	259	PHE
1	D	351	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	351	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	165	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 44 ligands modelled in this entry, 10 are monoatomic and 4 are unknown - leaving 30 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	$\# Z  > 2$
10	EDO	A	517	-	3,3,3	0.72	0	2,2,2	0.28	0
10	EDO	C	510	-	3,3,3	0.56	0	2,2,2	0.36	0
8	PEG	B	506	-	6,6,6	0.15	0	5,5,5	0.03	0
3	ADP	A	502	4	24,29,29	0.66	0	29,45,45	0.71	1 (3%)
10	EDO	D	506	-	3,3,3	0.53	0	2,2,2	0.35	0
10	EDO	D	507	-	3,3,3	0.60	0	2,2,2	0.32	0
6	SO4	B	504	-	4,4,4	0.10	0	6,6,6	0.08	0
7	PG4	A	510	-	12,12,12	0.21	0	11,11,11	0.05	0
6	SO4	A	507	-	4,4,4	0.17	0	6,6,6	0.07	0
9	PGE	A	512	-	9,9,9	0.19	0	8,8,8	0.04	0
3	ADP	D	501	-	24,29,29	0.63	0	29,45,45	0.70	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	EDO	C	509	-	3,3,3	0.62	0	2,2,2	0.32	0
6	SO4	A	508	-	4,4,4	0.15	0	6,6,6	0.05	0
6	SO4	B	505	-	4,4,4	0.10	0	6,6,6	0.06	0
10	EDO	B	507	-	3,3,3	0.60	0	2,2,2	0.31	0
9	PGE	C	507	-	9,9,9	0.14	0	8,8,8	0.07	0
8	PEG	A	511	-	6,6,6	0.18	0	5,5,5	0.02	0
10	EDO	A	516	-	3,3,3	0.52	0	2,2,2	0.32	0
6	SO4	C	506	-	4,4,4	0.11	0	6,6,6	0.08	0
10	EDO	A	513	-	3,3,3	0.59	0	2,2,2	0.32	0
3	ADP	B	502	-	24,29,29	0.71	0	29,45,45	0.69	1 (3%)
6	SO4	A	509	-	4,4,4	0.16	0	6,6,6	0.06	0
10	EDO	C	508	-	3,3,3	0.57	0	2,2,2	0.34	0
10	EDO	A	514	-	3,3,3	0.57	0	2,2,2	0.33	0
10	EDO	D	508	-	3,3,3	0.64	0	2,2,2	0.32	0
6	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.05	0
10	EDO	A	515	-	3,3,3	0.63	0	2,2,2	0.29	0
10	EDO	B	508	-	3,3,3	0.59	0	2,2,2	0.34	0
10	EDO	B	509	-	3,3,3	0.58	0	2,2,2	0.33	0
3	ADP	C	502	4	24,29,29	0.70	0	29,45,45	0.70	1 (3%)

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
10	EDO	A	517	-	-	0/1/1/1	-
10	EDO	C	510	-	-	0/1/1/1	-
8	PEG	B	506	-	-	2/4/4/4	-
3	ADP	A	502	4	-	1/12/32/32	0/3/3/3
10	EDO	D	506	-	-	0/1/1/1	-
10	EDO	D	507	-	-	0/1/1/1	-
7	PG4	A	510	-	-	1/10/10/10	-
9	PGE	A	512	-	-	2/7/7/7	-
3	ADP	D	501	-	-	0/12/32/32	0/3/3/3
10	EDO	C	509	-	-	0/1/1/1	-
10	EDO	B	507	-	-	0/1/1/1	-
9	PGE	C	507	-	-	4/7/7/7	-
8	PEG	A	511	-	-	1/4/4/4	-
10	EDO	A	516	-	-	0/1/1/1	-
10	EDO	A	513	-	-	0/1/1/1	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	B	502	-	-	2/12/32/32	0/3/3/3
10	EDO	C	508	-	-	0/1/1/1	-
10	EDO	A	514	-	-	0/1/1/1	-
10	EDO	D	508	-	-	0/1/1/1	-
10	EDO	A	515	-	-	0/1/1/1	-
10	EDO	B	508	-	-	0/1/1/1	-
10	EDO	B	509	-	-	0/1/1/1	-
3	ADP	C	502	4	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	ADP	C5-C6-N6	2.32	123.87	120.35
3	D	501	ADP	C5-C6-N6	2.30	123.84	120.35
3	A	502	ADP	C5-C6-N6	2.30	123.84	120.35
3	B	502	ADP	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (15) torsion outliers are listed below:

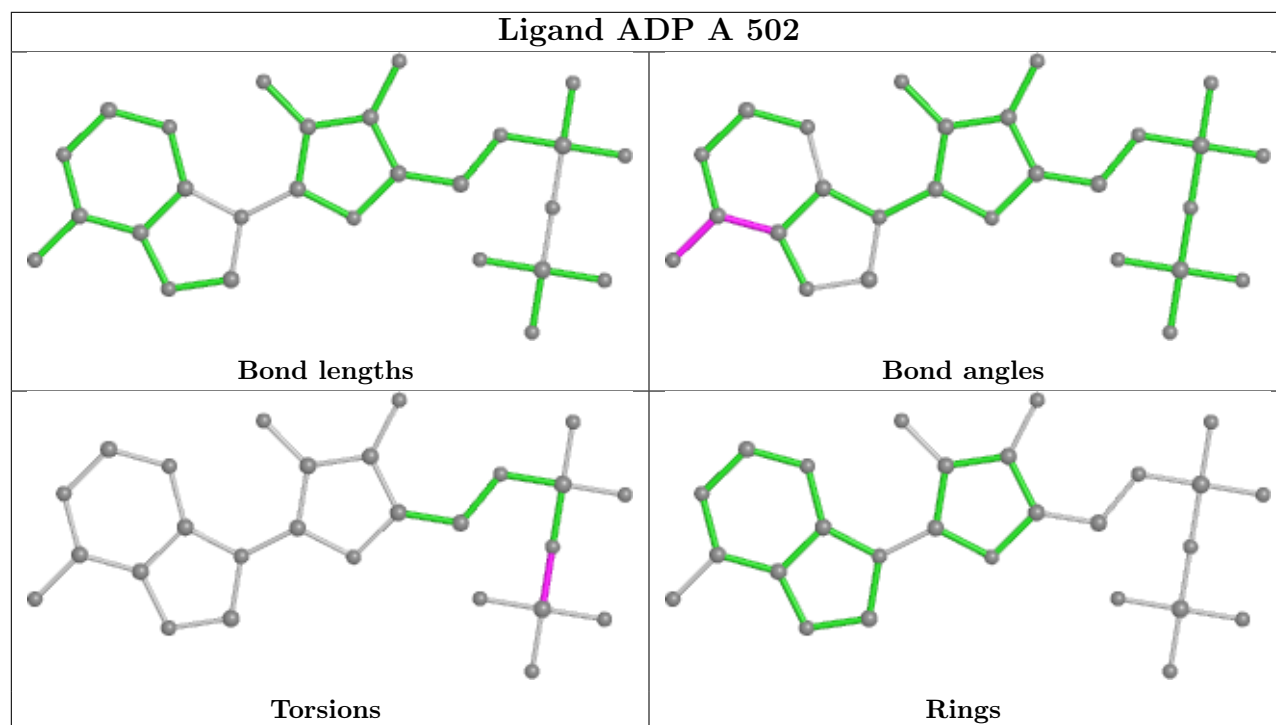
Mol	Chain	Res	Type	Atoms
3	B	502	ADP	PA-O3A-PB-O2B
3	B	502	ADP	PA-O3A-PB-O3B
9	A	512	PGE	C4-C3-O2-C2
7	A	510	PG4	C3-C4-O3-C5
3	C	502	ADP	PA-O3A-PB-O3B
9	C	507	PGE	C3-C4-O3-C5
9	C	507	PGE	C1-C2-O2-C3
9	C	507	PGE	C6-C5-O3-C4
8	B	506	PEG	C4-C3-O2-C2
8	A	511	PEG	C4-C3-O2-C2
9	A	512	PGE	C3-C4-O3-C5
3	A	502	ADP	PA-O3A-PB-O2B
3	C	502	ADP	PA-O3A-PB-O2B
9	C	507	PGE	O2-C3-C4-O3
8	B	506	PEG	C1-C2-O2-C3

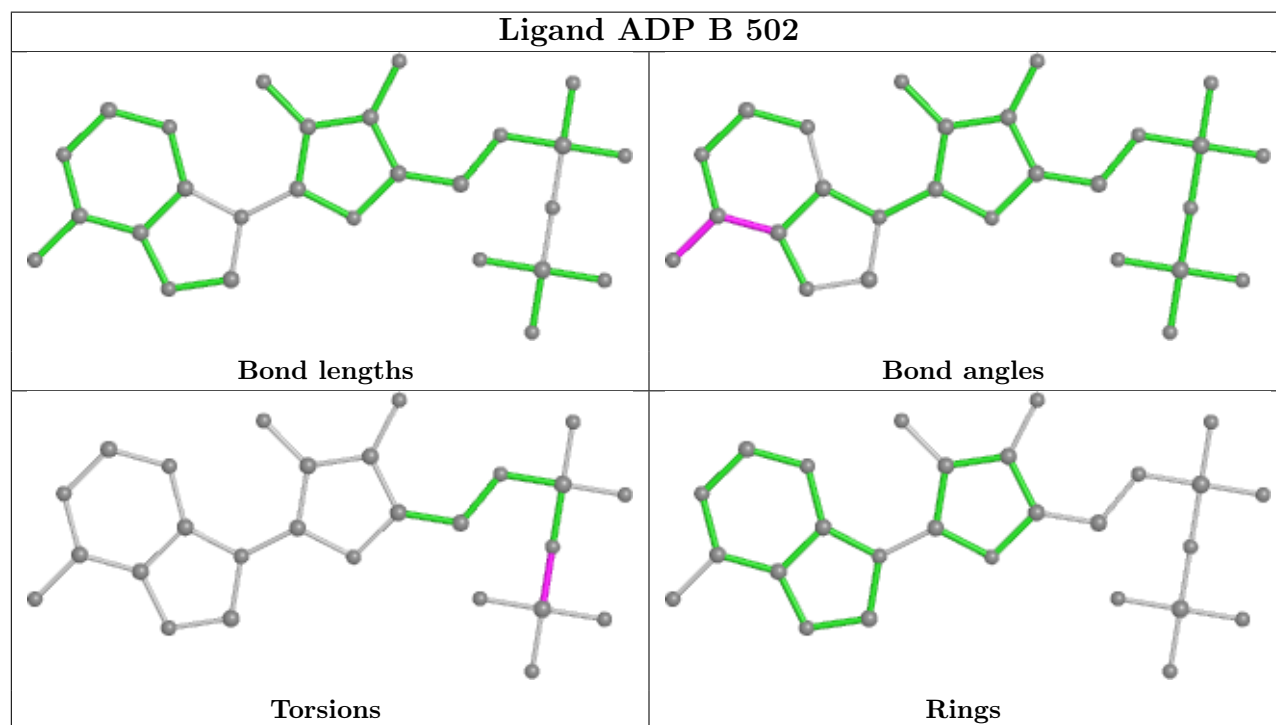
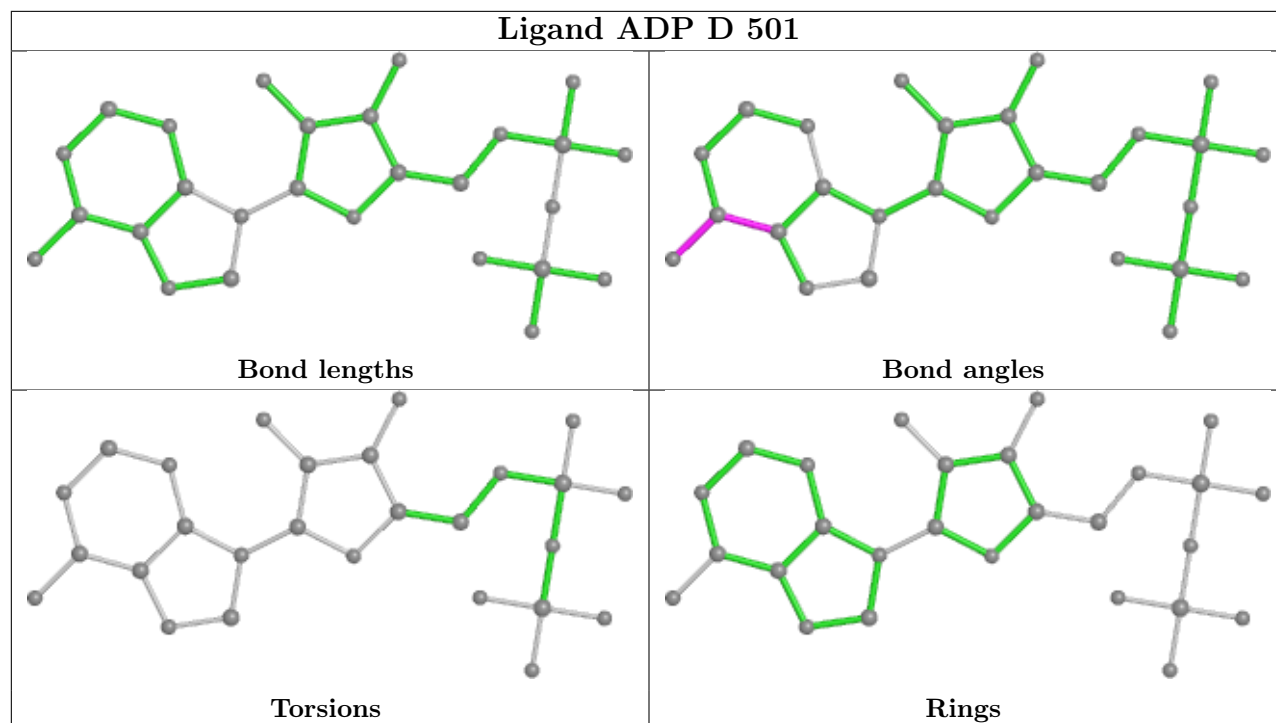
There are no ring outliers.

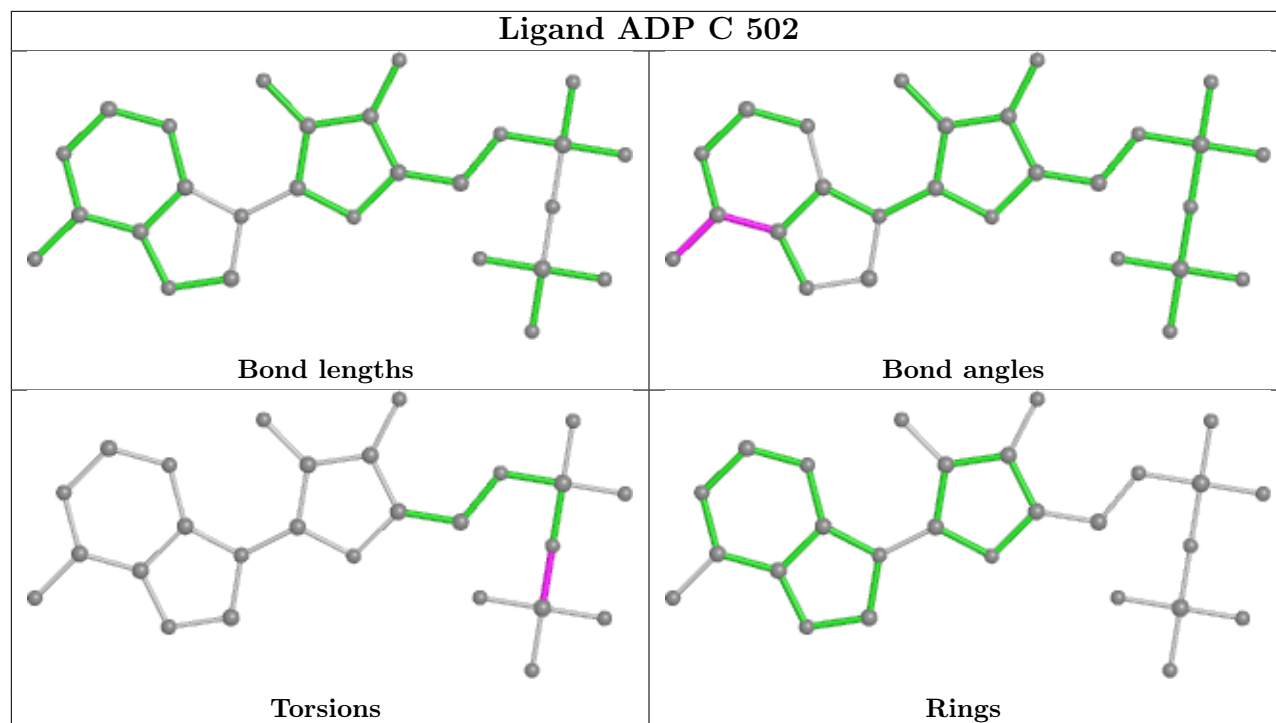
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ADP	1	0
3	D	501	ADP	1	0
3	C	502	ADP	1	0

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







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/436 (96%)	-0.02	13 (3%)	49 46	31, 50, 93, 115	0
1	B	414/436 (94%)	0.31	36 (8%)	10 9	32, 54, 96, 117	0
1	C	419/436 (96%)	0.11	12 (2%)	51 49	35, 58, 93, 114	0
1	D	414/436 (94%)	0.17	25 (6%)	21 20	31, 51, 93, 118	0
All	All	1666/1744 (95%)	0.14	86 (5%)	27 25	31, 53, 94, 118	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	ASN	6.1
1	A	426	VAL	5.1
1	A	427	ARG	4.6
1	D	338	VAL	4.3
1	B	369	GLN	4.2
1	D	367	ASN	4.1
1	B	382	SER	4.1
1	D	405	LEU	4.1
1	D	366	VAL	4.0
1	A	369	GLN	3.9
1	B	400	LEU	3.6
1	B	338	VAL	3.6
1	D	400	LEU	3.5
1	D	384	ASP	3.5
1	B	334	ILE	3.5
1	D	383	THR	3.4
1	A	97	THR	3.4
1	C	421	SER	3.4
1	D	398	ARG	3.3
1	A	421	SER	3.3
1	D	382	SER	3.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	431	LEU	3.2
1	B	371	GLU	3.1
1	B	368	ASN	3.1
1	B	404	ILE	3.1
1	C	53	ILE	3.1
1	B	370	ASP	3.0
1	B	340	ILE	3.0
1	D	363	LEU	3.0
1	D	94	SER	3.0
1	A	383	THR	3.0
1	A	425	ALA	3.0
1	A	0	GLY	3.0
1	D	396	ILE	2.9
1	C	0	GLY	2.9
1	B	431	LEU	2.9
1	C	426	VAL	2.9
1	B	339	ASN	2.9
1	B	335	ILE	2.8
1	B	407	THR	2.8
1	B	3	THR	2.7
1	C	383	THR	2.7
1	C	16	GLU	2.7
1	B	364	GLU	2.6
1	D	373	ILE	2.6
1	D	335	ILE	2.5
1	B	97	THR	2.5
1	A	384	ASP	2.5
1	C	423	GLY	2.5
1	B	333	PHE	2.5
1	D	397	ILE	2.5
1	B	422	GLU	2.5
1	B	379	SER	2.5
1	A	422	GLU	2.5
1	D	352	PHE	2.4
1	B	196	GLN	2.4
1	C	54	GLN	2.4
1	B	363	LEU	2.4
1	D	355	LEU	2.4
1	B	396	ILE	2.4
1	B	413	VAL	2.4
1	B	403	GLU	2.4
1	A	420	GLN	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	49	THR	2.4
1	B	373	ILE	2.3
1	D	402	ASP	2.3
1	B	432	ARG	2.3
1	D	380	ASP	2.3
1	B	406	VAL	2.3
1	D	374	VAL	2.3
1	B	384	ASP	2.3
1	C	18	LEU	2.3
1	D	369	GLN	2.2
1	D	404	ILE	2.2
1	D	406	VAL	2.2
1	D	334	ILE	2.2
1	B	272	GLU	2.2
1	B	348	ILE	2.1
1	C	57	ASP	2.1
1	B	398	ARG	2.1
1	B	199	GLY	2.1
1	A	428	VAL	2.0
1	B	386	TYR	2.0
1	C	145	LEU	2.0
1	B	94	SER	2.0
1	B	337	GLY	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 monosaccharides 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, 95<sup>th</sup> 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.

*Continued on next page...*

*Continued from previous page...*

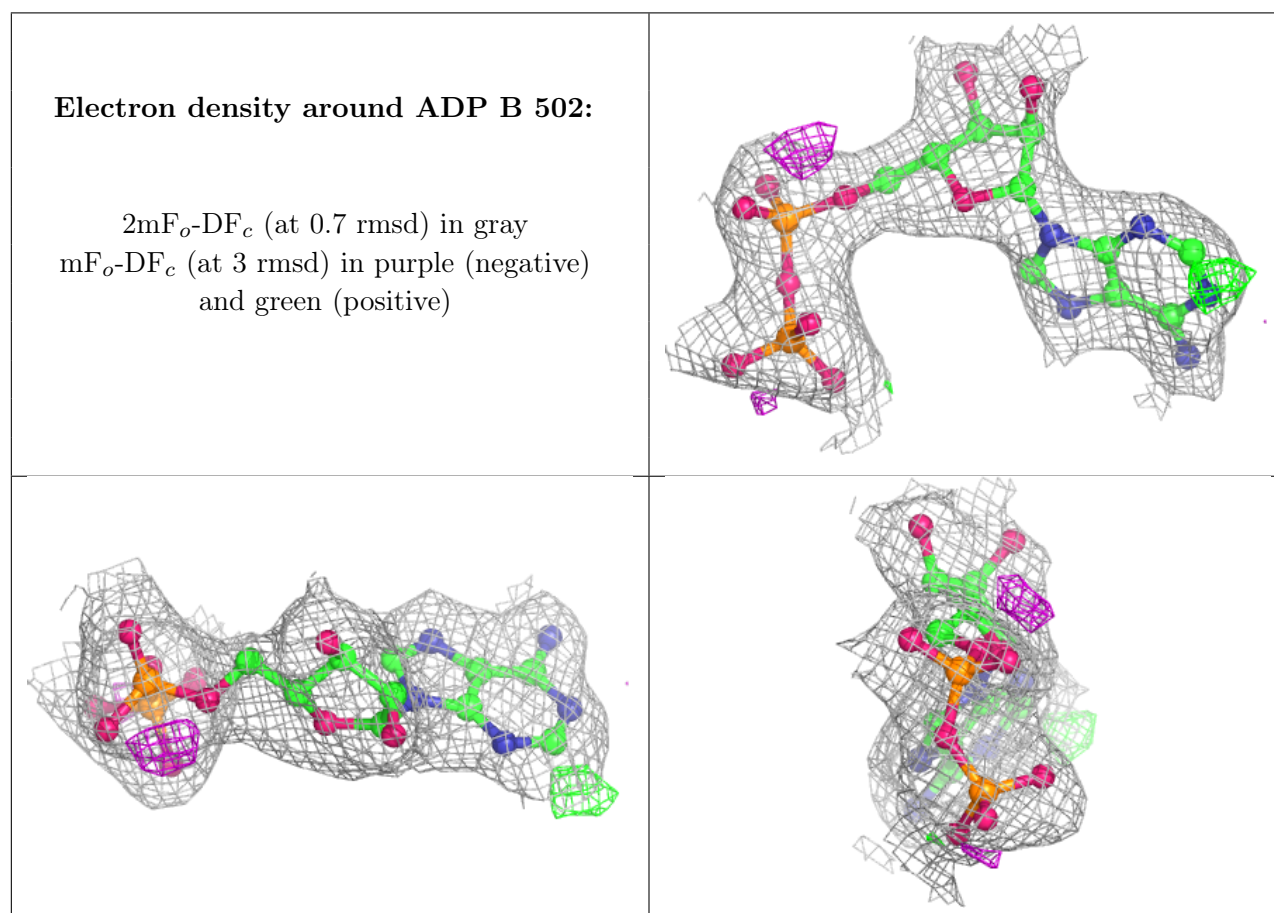
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	EDO	A	517	4/4	0.63	0.30	64,65,66,66	0
9	PGE	A	512	10/10	0.66	0.31	87,88,88,89	0
10	EDO	A	513	4/4	0.73	0.25	73,73,74,74	0
10	EDO	A	515	4/4	0.76	0.18	62,63,64,64	0
9	PGE	C	507	10/10	0.76	0.22	55,67,77,77	0
7	PG4	A	510	13/13	0.82	0.19	64,66,69,69	0
10	EDO	B	507	4/4	0.82	0.26	80,80,80,81	0
5	UNL	C	505	13/-	0.85	0.41	35,51,66,66	0
5	UNL	A	506	7/-	0.85	0.49	29,33,50,57	0
10	EDO	B	509	4/4	0.85	0.19	64,64,64,65	0
10	EDO	C	509	4/4	0.88	0.22	59,60,60,60	0
8	PEG	B	506	7/7	0.89	0.13	58,59,63,64	0
6	SO4	A	509	5/5	0.89	0.13	101,102,102,103	0
8	PEG	A	511	7/7	0.89	0.14	51,54,56,56	0
6	SO4	B	504	5/5	0.90	0.16	85,86,88,88	0
10	EDO	B	508	4/4	0.90	0.21	64,64,64,64	0
10	EDO	D	506	4/4	0.90	0.19	42,44,45,45	0
5	UNL	D	504	9/-	0.91	0.36	33,44,52,53	0
6	SO4	A	508	5/5	0.91	0.15	89,89,90,90	0
10	EDO	A	514	4/4	0.91	0.17	53,53,55,56	0
5	UNL	B	503	8/-	0.91	0.28	23,30,46,82	0
4	K	D	503	1/1	0.91	0.09	42,42,42,42	0
10	EDO	D	508	4/4	0.91	0.13	57,59,61,62	0
10	EDO	C	508	4/4	0.92	0.12	54,54,55,56	0
6	SO4	B	505	5/5	0.92	0.14	94,95,96,96	0
10	EDO	D	507	4/4	0.93	0.28	48,48,50,51	0
6	SO4	C	506	5/5	0.93	0.16	79,81,81,83	0
3	ADP	B	502	27/27	0.94	0.15	43,48,56,58	0
10	EDO	C	510	4/4	0.94	0.11	54,55,56,57	0
3	ADP	C	502	27/27	0.94	0.16	42,44,57,59	0
10	EDO	A	516	4/4	0.94	0.27	59,60,60,61	0
2	ZN	C	501	1/1	0.94	0.07	58,58,58,58	0
3	ADP	D	501	27/27	0.95	0.14	37,45,63,67	0
3	ADP	A	502	27/27	0.95	0.14	21,36,54,56	0
6	SO4	D	505	5/5	0.96	0.14	70,71,72,75	0
4	K	A	503	1/1	0.96	0.07	49,49,49,49	0
2	ZN	D	502	1/1	0.97	0.06	40,40,40,40	0
2	ZN	B	501	1/1	0.97	0.06	39,39,39,39	0
6	SO4	A	507	5/5	0.97	0.15	54,56,56,59	0
4	K	C	504	1/1	0.97	0.08	38,38,38,38	0
4	K	C	503	1/1	0.98	0.09	54,54,54,54	0

*Continued on next page...*

*Continued from previous page...*

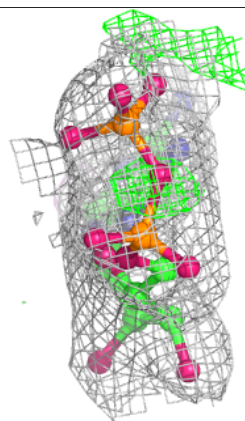
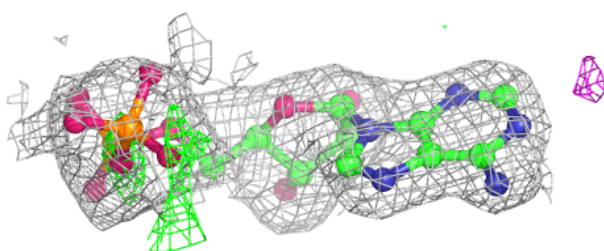
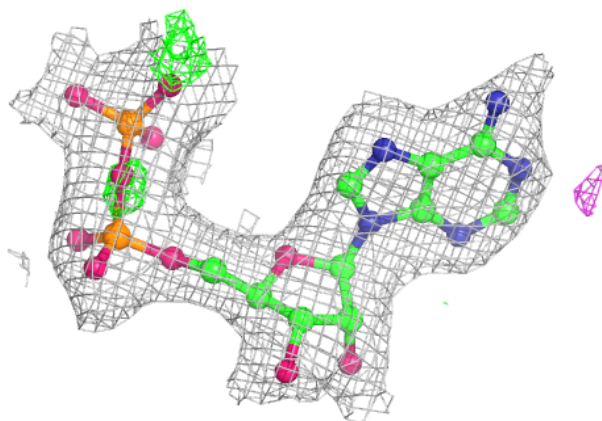
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	A	501	1/1	0.98	0.09	42,42,42,42	0
4	K	A	504	1/1	0.98	0.08	42,42,42,42	0
4	K	A	505	1/1	0.99	0.06	29,29,29,29	0

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.



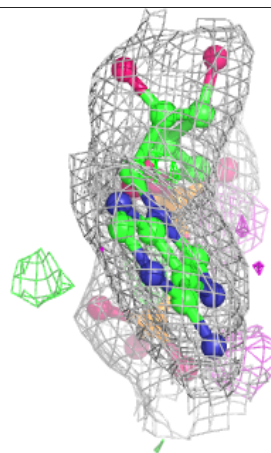
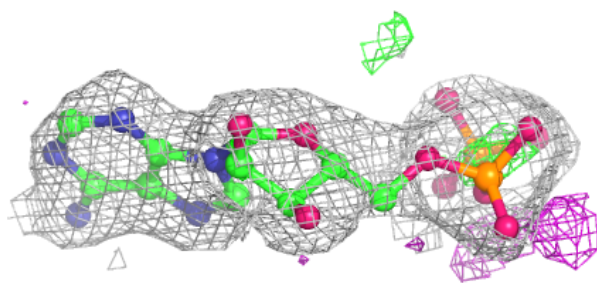
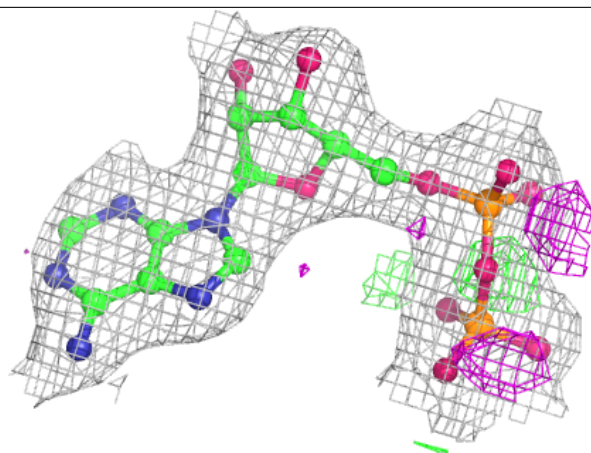
**Electron density around ADP C 502:**

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



**Electron density around ADP D 501:**

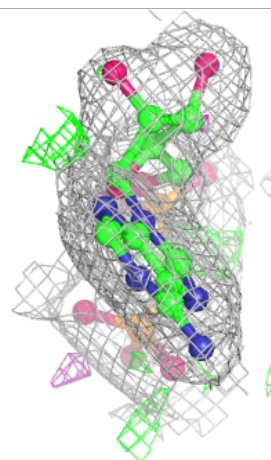
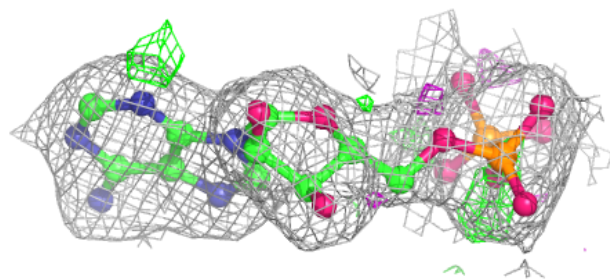
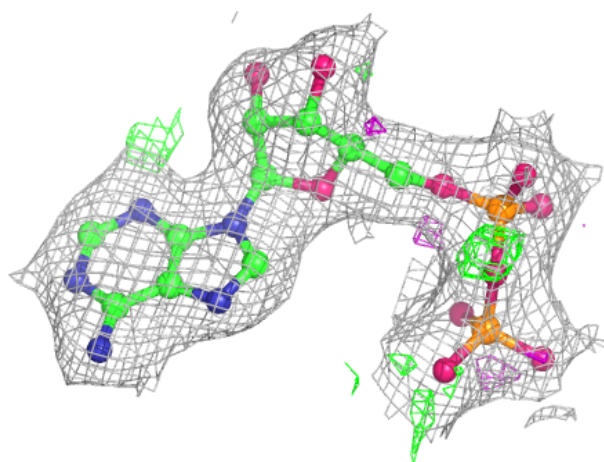
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around ADP A 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.