



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 08:11 AM BST

PDB ID : 5UYX  
Title : Structure of Human T-complex protein 1 subunit epsilon (CCT5)  
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Deposited on : 2017-02-24  
Resolution : 3.50 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.

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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	:	2.13.1
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)	:	2.13.1

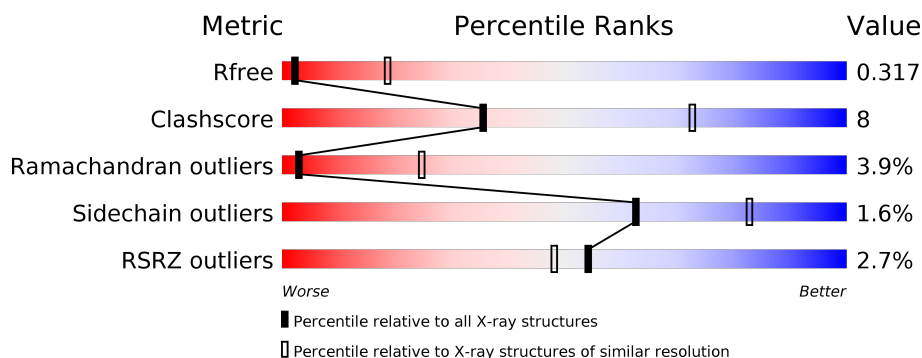
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	541	<div> <div>3%</div> <div> <div></div> <div>68%</div> <div>21%</div> <div>• 9%</div> </div> </div>
1	B	541	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>18%</div> <div>• 11%</div> </div> </div>
1	C	541	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>• 12%</div> </div> </div>
1	D	541	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>18%</div> <div>• 17%</div> </div> </div>

## 2 Entry composition [i](#)

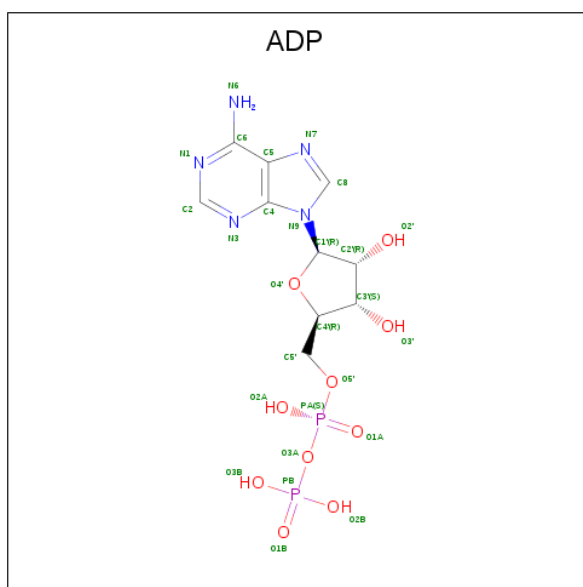
There are 2 unique types of molecules in this entry. The entry contains 14749 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 T-complex protein 1 subunit epsilon.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3787	2374	656	729	28			
1	B	484	Total	C	N	O	S	0	0	0
			3726	2335	647	716	28			
1	C	474	Total	C	N	O	S	0	0	0
			3658	2296	635	701	26			
1	D	451	Total	C	N	O	S	0	0	0
			3470	2180	595	669	26			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



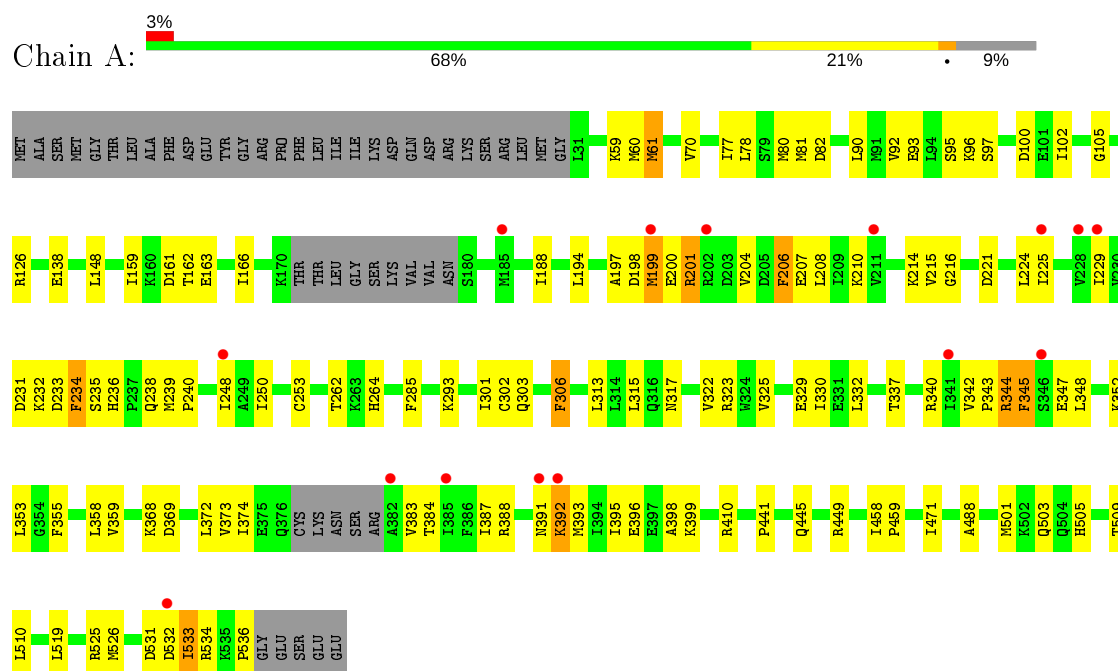
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

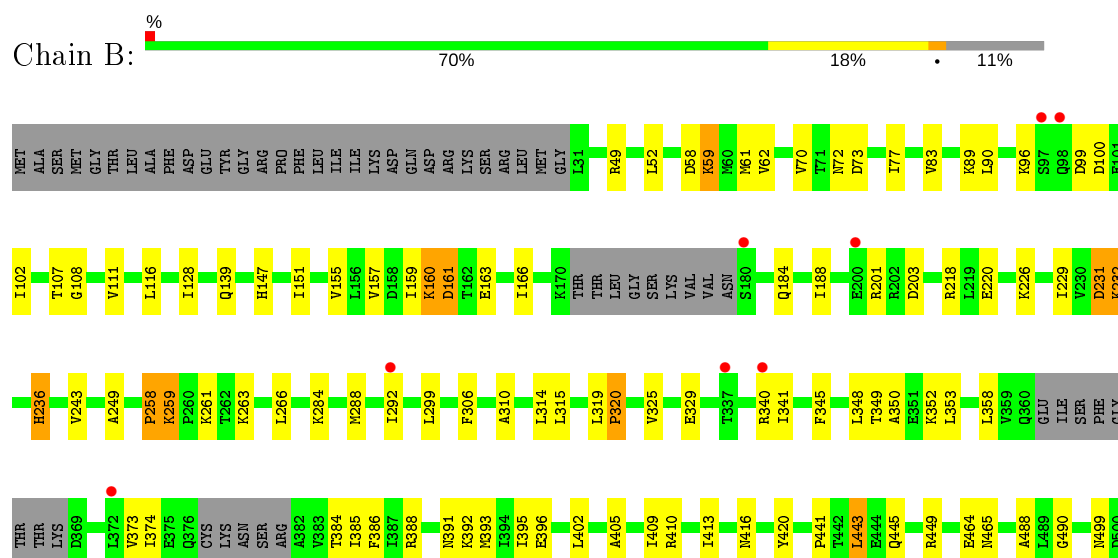
### 3 Residue-property plots

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: T-complex protein 1 subunit epsilon

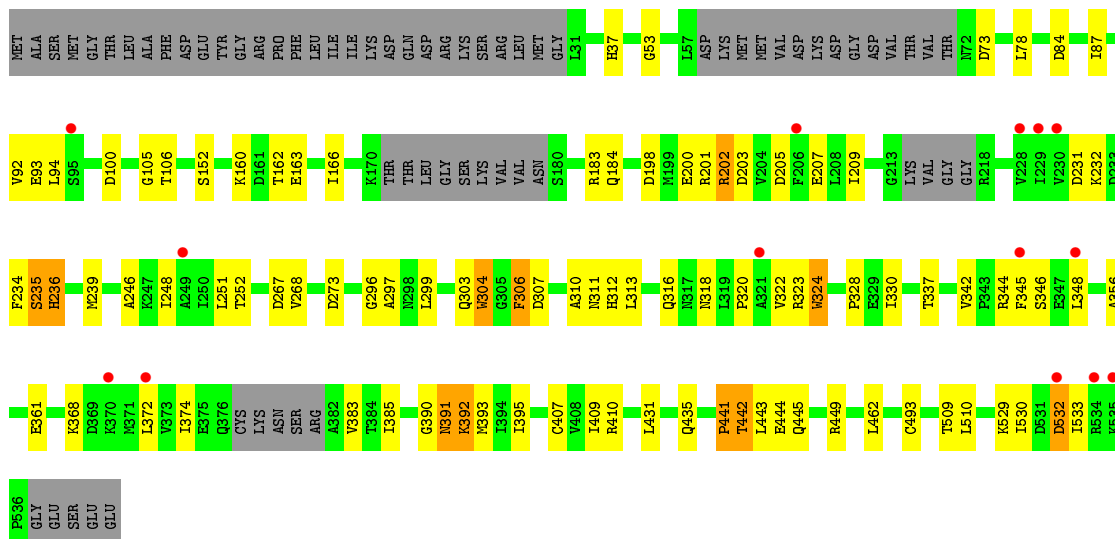


#### • Molecule 1: T-complex protein 1 subunit epsilon

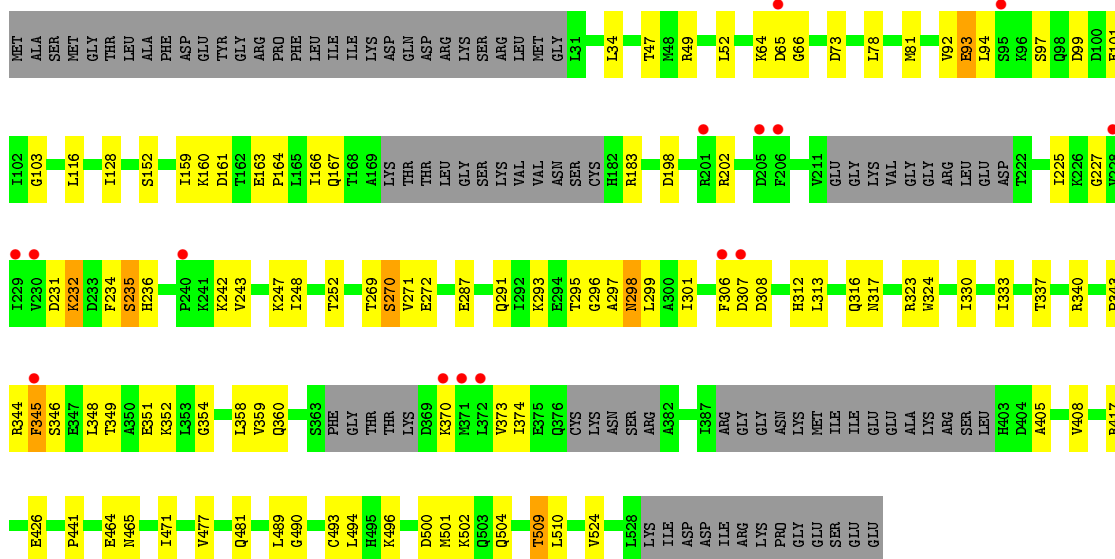




- Molecule 1: T-complex protein 1 subunit epsilon



- Molecule 1: T-complex protein 1 subunit epsilon



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.71Å 204.71Å 162.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.70 – 3.50 75.70 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (75.70-3.50) 99.7 (75.70-3.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.49Å)	Xtriage
Refinement program	PHENIX (dev_2650: ???)	Depositor
R, $R_{free}$	0.269 , 0.318 0.268 , 0.317	Depositor DCC
$R_{free}$ test set	2216 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	114.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14749	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	124.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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

### 5.1 Standard geometry

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	0.24	0/3831	0.44	0/5162
1	B	0.24	0/3768	0.43	0/5076
1	C	0.24	0/3700	0.44	0/4984
1	D	0.24	0/3509	0.43	0/4733
All	All	0.24	0/14808	0.43	0/19955

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	161	ASP	Peptide
1	D	161	ASP	Peptide



## 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	3787	0	3890	66	0
1	B	3726	0	3828	66	0
1	C	3658	0	3756	60	0
1	D	3470	0	3550	57	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
All	All	14749	0	15072	241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:NZ	1:A:369:ASP:OD2	2.02	0.92
1:A:199:MET:O	1:A:201:ARG:NH1	2.07	0.87
1:A:96:LYS:NZ	1:A:100:ASP:OD2	2.09	0.83
1:A:93:GLU:O	1:A:97:SER:HB3	1.80	0.82
1:A:293:LYS:NZ	1:A:317:ASN:O	2.12	0.81
1:B:96:LYS:NZ	1:B:100:ASP:OD2	2.15	0.79
1:A:262:THR:O	1:A:264:HIS:ND1	2.19	0.75
1:C:198:ASP:OD1	1:C:200:GLU:OE2	2.03	0.75
1:C:201:ARG:O	1:C:203:ASP:N	2.22	0.73
1:C:209:ILE:HD13	1:C:383:VAL:HG13	1.73	0.70
1:A:198:ASP:O	1:A:200:GLU:N	2.26	0.69
1:D:92:VAL:O	1:D:94:LEU:N	2.23	0.68
1:C:198:ASP:OD1	1:C:202:ARG:NH1	2.27	0.68
1:C:246:ALA:HB3	1:C:356:ALA:HB3	1.76	0.68
1:D:247:LYS:H	1:D:298:ASN:HB2	1.58	0.68
1:A:250:ILE:HG23	1:A:301:ILE:HD11	1.74	0.67
1:C:198:ASP:CG	1:C:200:GLU:OE2	2.33	0.67
1:D:92:VAL:HG12	1:D:93:GLU:H	1.61	0.66
1:A:313:LEU:O	1:A:317:ASN:ND2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HH12	1:B:353:LEU:HD12	1.61	0.65
1:B:218:ARG:O	1:B:220:GLU:N	2.26	0.64
1:D:198:ASP:OD2	1:D:202:ARG:HG2	1.97	0.64
1:A:391:ASN:O	1:A:393:MET:N	2.32	0.63
1:A:303:GLN:HB2	1:A:330:ILE:HD11	1.82	0.62
1:A:206:PHE:HD1	1:A:207:GLU:HG2	1.63	0.62
1:A:359:VAL:HG22	1:A:372:LEU:HD22	1.81	0.61
1:B:163:GLU:O	1:B:166:ILE:N	2.25	0.61
1:B:259:LYS:H	1:B:259:LYS:HD3	1.67	0.60
1:B:490:GLY:O	1:B:499:ASN:ND2	2.35	0.60
1:C:310:ALA:HA	1:C:313:LEU:HD12	1.82	0.60
1:D:293:LYS:HA	1:D:297:ALA:HB2	1.82	0.60
1:C:78:LEU:HD22	1:C:92:VAL:HG22	1.84	0.60
1:C:312:HIS:O	1:C:316:GLN:HG2	2.03	0.59
1:C:361:GLU:OE2	1:C:368:LYS:HE2	2.03	0.58
1:C:445:GLN:OE1	1:C:449:ARG:NH2	2.37	0.58
1:D:297:ALA:O	1:D:299:LEU:N	2.37	0.58
1:D:64:LYS:O	1:D:66:GLY:N	2.37	0.57
1:C:306:PHE:HB2	1:C:310:ALA:HB3	1.85	0.57
1:D:481:GLN:NE2	1:D:489:LEU:O	2.36	0.57
1:C:163:GLU:OE2	1:C:183:ARG:NE	2.38	0.57
1:B:306:PHE:HB3	1:B:310:ALA:HB3	1.86	0.57
1:C:303:GLN:HB2	1:C:330:ILE:HD11	1.85	0.57
1:C:209:ILE:HD11	1:C:385:ILE:HG13	1.87	0.56
1:A:102:ILE:O	1:A:410:ARG:NH2	2.38	0.56
1:B:258:PRO:HG2	1:B:284:LYS:HD2	1.86	0.56
1:B:340:ARG:NH2	1:B:349:THR:O	2.39	0.56
1:C:152:SER:HB3	1:C:510:LEU:HD12	1.87	0.56
1:B:350:ALA:HA	1:B:353:LEU:HD13	1.88	0.55
1:A:348:LEU:HD12	1:A:353:LEU:HD21	1.89	0.55
1:A:358:LEU:HB3	1:A:373:VAL:HG23	1.89	0.55
1:B:340:ARG:HH12	1:B:353:LEU:CD1	2.19	0.54
1:D:500:ASP:OD2	1:D:502:LYS:HB2	2.07	0.54
1:D:252:THR:HG22	1:D:330:ILE:HD13	1.90	0.54
1:D:93:GLU:O	1:D:97:SER:OG	2.20	0.53
1:A:210:LYS:HE3	1:A:329:GLU:HG3	1.91	0.53
1:D:501:MET:HA	1:D:504:GLN:HB2	1.88	0.53
1:A:250:ILE:HA	1:A:301:ILE:HG13	1.90	0.53
1:D:231:ASP:O	1:D:370:LYS:NZ	2.42	0.52
1:B:58:ASP:HB3	1:B:70:VAL:HG13	1.91	0.52
1:C:431:LEU:O	1:C:435:GLN:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:VAL:HB	1:D:359:VAL:HG13	1.89	0.52
1:B:243:VAL:HG21	1:B:299:LEU:HD12	1.90	0.52
1:A:163:GLU:OE1	1:A:163:GLU:N	2.39	0.52
1:B:229:ILE:HG22	1:B:384:THR:HG21	1.92	0.52
1:C:532:ASP:OD2	1:D:47:THR:HG23	2.09	0.52
1:A:198:ASP:OD2	1:A:204:VAL:N	2.40	0.52
1:D:242:LYS:HG3	1:D:360:GLN:HB3	1.90	0.52
1:A:236:HIS:CE1	1:A:315:LEU:HD22	2.44	0.52
1:C:100:ASP:OD1	1:C:106:THR:OG1	2.29	0.51
1:B:340:ARG:HH22	1:B:353:LEU:HD12	1.76	0.51
1:C:442:THR:O	1:C:444:GLU:N	2.44	0.51
1:B:157:VAL:HG11	1:B:413:ILE:HG12	1.92	0.51
1:D:163:GLU:OE2	1:D:183:ARG:NE	2.44	0.51
1:B:259:LYS:H	1:B:259:LYS:CD	2.24	0.51
1:A:90:LEU:HD21	1:A:526:MET:HE2	1.92	0.51
1:C:92:VAL:HG12	1:C:93:GLU:H	1.76	0.50
1:C:235:SER:OG	1:C:311:ASN:ND2	2.44	0.50
1:B:163:GLU:OE1	1:B:163:GLU:N	2.32	0.50
1:B:90:LEU:HD21	1:B:526:MET:HE2	1.93	0.50
1:C:328:PRO:C	1:C:330:ILE:H	2.15	0.50
1:C:307:ASP:HA	1:C:323:ARG:HH22	1.75	0.50
1:D:307:ASP:HB2	1:D:324:TRP:HH2	1.75	0.50
1:C:53:GLY:N	2:C:601:ADP:O2A	2.42	0.50
1:B:395:ILE:HG22	1:B:396:GLU:H	1.77	0.50
1:C:198:ASP:O	1:C:200:GLU:OE1	2.30	0.50
1:A:303:GLN:HG3	1:A:325:VAL:O	2.12	0.49
1:A:344:ARG:HD2	1:A:347:GLU:HB2	1.94	0.49
1:C:234:PHE:HE2	1:C:361:GLU:HB2	1.77	0.49
1:A:264:HIS:HB3	1:B:266:LEU:HD23	1.93	0.49
1:C:200:GLU:H	1:C:200:GLU:CD	2.16	0.49
1:D:232:LYS:O	1:D:370:LYS:NZ	2.35	0.49
1:A:206:PHE:HD1	1:A:207:GLU:H	1.61	0.49
1:A:445:GLN:OE1	1:A:449:ARG:NH2	2.45	0.49
1:A:61:MET:HE1	1:A:77:ILE:HA	1.94	0.49
1:B:288:MET:O	1:B:292:ILE:HG12	2.13	0.49
1:C:267:ASP:HB2	1:D:269:THR:HG22	1.95	0.49
1:A:159:ILE:O	1:A:161:ASP:N	2.46	0.49
1:D:295:THR:O	1:D:297:ALA:N	2.46	0.49
1:C:234:PHE:HB3	1:C:322:VAL:HG22	1.95	0.49
1:A:340:ARG:HB2	1:A:352:LYS:HB3	1.94	0.49
1:B:128:ILE:HG12	1:B:443:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:SER:OG	1:D:323:ARG:NE	2.45	0.48
1:D:351:GLU:OE1	1:D:351:GLU:N	2.45	0.48
1:A:488:ALA:O	1:A:501:MET:N	2.32	0.48
1:D:494:LEU:HB2	1:D:496:LYS:HG2	1.94	0.48
1:A:229:ILE:N	1:A:384:THR:HG21	2.28	0.48
1:B:236:HIS:NE2	1:B:315:LEU:HD22	2.28	0.48
1:C:252:THR:HG22	1:C:330:ILE:HD13	1.96	0.48
1:B:49:ARG:NH1	1:B:464:GLU:OE1	2.38	0.48
1:C:407:CYS:SG	1:C:410:ARG:NH2	2.87	0.48
1:D:152:SER:HB3	1:D:510:LEU:HD13	1.95	0.48
1:A:392:LYS:HG3	1:A:393:MET:HG3	1.95	0.47
1:B:107:THR:HB	2:B:601:ADP:O1B	2.14	0.47
1:A:60:MET:HA	1:A:70:VAL:HG22	1.95	0.47
1:C:303:GLN:HA	1:C:324:TRP:HA	1.96	0.47
1:C:268:VAL:HG13	1:C:273:ASP:HB2	1.97	0.47
1:C:303:GLN:O	1:C:304:TRP:HB2	2.14	0.47
1:A:224:LEU:HG	1:A:225:ILE:H	1.79	0.47
1:B:391:ASN:O	1:B:393:MET:N	2.46	0.47
1:C:239:MET:SD	1:C:320:PRO:HA	2.54	0.47
1:D:52:LEU:O	1:D:465:ASN:ND2	2.45	0.47
1:A:306:PHE:CD1	1:A:323:ARG:HB3	2.50	0.47
1:C:166:ILE:HD11	1:C:409:ILE:HG13	1.97	0.47
1:C:441:PRO:HG2	1:C:442:THR:HG23	1.96	0.47
1:D:164:PRO:O	1:D:167:GLN:HB2	2.13	0.47
1:A:78:LEU:HD22	1:A:92:VAL:HG22	1.96	0.47
1:B:288:MET:HG2	1:B:345:PHE:CZ	2.50	0.47
1:D:49:ARG:NH1	1:D:464:GLU:OE1	2.48	0.47
1:B:443:LEU:H	1:B:443:LEU:HD12	1.79	0.47
1:B:358:LEU:HB3	1:B:373:VAL:HG23	1.97	0.47
1:D:293:LYS:HA	1:D:297:ALA:CB	2.44	0.47
1:D:345:PHE:O	1:D:345:PHE:CG	2.68	0.46
1:A:387:ILE:HD11	1:A:398:ALA:HB3	1.96	0.46
1:D:99:ASP:O	1:D:103:GLY:N	2.40	0.46
1:B:503:GLN:C	1:B:505:HIS:H	2.17	0.46
1:A:234:PHE:O	1:A:322:VAL:HA	2.14	0.46
1:A:531:ASP:O	1:B:59:LYS:HA	2.15	0.46
1:A:225:ILE:HD12	1:A:383:VAL:HG21	1.97	0.46
1:A:229:ILE:H	1:A:384:THR:HG21	1.81	0.46
1:A:221:ASP:HB2	1:A:388:ARG:HB2	1.97	0.46
1:A:162:THR:O	1:A:166:ILE:HG12	2.16	0.46
1:B:61:MET:HE1	1:B:77:ILE:HA	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:ILE:O	1:D:354:GLY:N	2.47	0.46
1:D:349:THR:OG1	1:D:351:GLU:OE1	2.23	0.46
1:D:159:ILE:HG13	1:D:160:LYS:H	1.80	0.46
1:A:248:ILE:HD12	1:A:337:THR:HG21	1.97	0.45
1:B:386:PHE:CE2	1:B:388:ARG:HD3	2.51	0.45
1:D:426:GLU:N	1:D:426:GLU:OE1	2.44	0.45
1:D:333:ILE:O	1:D:337:THR:HG22	2.15	0.45
1:B:340:ARG:HB3	1:B:352:LYS:HB3	1.98	0.45
1:C:307:ASP:HA	1:C:323:ARG:NH2	2.32	0.45
1:C:390:GLY:C	1:C:392:LYS:H	2.20	0.45
1:C:344:ARG:NH1	1:D:307:ASP:OD2	2.49	0.45
1:C:342:VAL:HG11	1:C:348:LEU:HB3	1.98	0.45
1:B:340:ARG:NH1	1:B:353:LEU:HA	2.30	0.45
1:C:84:ASP:OD1	1:C:84:ASP:N	2.48	0.45
1:D:101:GLU:OE1	1:D:101:GLU:N	2.50	0.45
1:A:215:VAL:HA	1:A:395:ILE:HD12	1.99	0.44
1:A:536:PRO:HD2	1:B:62:VAL:O	2.17	0.44
1:D:301:ILE:HD12	1:D:333:ILE:HG21	1.99	0.44
1:B:385:ILE:HG21	1:B:402:LEU:HD21	1.99	0.44
1:A:216:GLY:O	1:A:388:ARG:NH2	2.51	0.44
1:A:138:GLU:HB2	1:A:525:ARG:HH22	1.81	0.44
1:D:312:HIS:O	1:D:316:GLN:HG2	2.17	0.44
1:A:503:GLN:C	1:A:505:HIS:H	2.21	0.44
1:A:188:ILE:HG12	1:A:224:LEU:HD13	2.00	0.44
1:C:345:PHE:O	1:C:345:PHE:CG	2.71	0.44
1:A:239:MET:HG3	1:A:240:PRO:HD2	2.00	0.44
1:B:155:VAL:O	1:B:416:ASN:HB2	2.18	0.44
1:B:231:ASP:N	1:B:231:ASP:OD1	2.36	0.44
1:B:184:GLN:O	1:B:188:ILE:HG12	2.18	0.43
1:B:531:ASP:OD1	1:B:531:ASP:N	2.52	0.43
1:D:477:VAL:HG11	1:D:490:GLY:HA2	2.00	0.43
1:D:344:ARG:O	1:D:346:SER:N	2.50	0.43
1:A:395:ILE:HG22	1:A:399:LYS:HD2	2.01	0.43
1:D:152:SER:HB2	1:D:417:ARG:HB3	2.00	0.43
1:B:263:LYS:H	1:B:263:LYS:HG3	1.64	0.43
1:A:458:ILE:HB	1:A:459:PRO:HD3	2.01	0.43
1:B:284:LYS:O	1:B:288:MET:HG3	2.18	0.43
1:C:391:ASN:C	1:C:393:MET:H	2.21	0.43
1:C:248:ILE:HD12	1:C:337:THR:HG21	2.00	0.43
1:A:253:CYS:SG	1:A:345:PHE:HA	2.58	0.43
1:D:116:LEU:HB2	1:D:524:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:VAL:C	1:D:94:LEU:H	2.17	0.43
1:C:306:PHE:HB2	1:C:310:ALA:CB	2.49	0.43
1:C:391:ASN:O	1:C:393:MET:N	2.52	0.43
1:A:342:VAL:HG11	1:A:348:LEU:HB3	2.00	0.42
1:C:207:GLU:OE1	1:C:410:ARG:NH1	2.52	0.42
1:A:233:ASP:HB3	1:A:368:LYS:HG3	2.01	0.42
1:B:249:ALA:HB1	1:B:348:LEU:HD11	2.02	0.42
1:B:116:LEU:HB2	1:B:524:VAL:HG21	2.02	0.42
1:A:138:GLU:OE1	1:A:525:ARG:NH2	2.53	0.42
1:D:358:LEU:HB3	1:D:373:VAL:HG23	2.00	0.42
1:B:340:ARG:NH2	1:B:352:LYS:HB2	2.35	0.42
1:B:420:TYR:CZ	1:B:502:LYS:HD3	2.54	0.42
1:C:236:HIS:HB2	1:C:311:ASN:OD1	2.20	0.42
1:B:102:ILE:O	1:B:410:ARG:NH2	2.52	0.42
1:C:462:LEU:HD22	1:C:493:CYS:SG	2.60	0.42
1:D:313:LEU:O	1:D:317:ASN:ND2	2.46	0.42
1:B:163:GLU:HA	1:B:166:ILE:HG12	2.02	0.41
1:A:302:CYS:O	1:A:303:GLN:HB3	2.20	0.41
1:B:108:GLY:HA2	1:B:111:VAL:HG12	2.02	0.41
1:C:105:GLY:HA2	2:C:601:ADP:PB	2.60	0.41
1:B:52:LEU:O	1:B:465:ASN:ND2	2.53	0.41
1:B:488:ALA:O	1:B:501:MET:N	2.41	0.41
1:C:160:LYS:O	1:C:162:THR:N	2.44	0.41
1:B:325:VAL:HG12	1:B:329:GLU:HB2	2.02	0.41
1:B:83:VAL:HG21	1:B:89:LYS:HA	2.02	0.41
1:B:231:ASP:HB2	1:B:232:LYS:H	1.72	0.41
1:B:405:ALA:O	1:B:409:ILE:HG13	2.21	0.41
1:C:395:ILE:H	1:C:395:ILE:HG12	1.69	0.41
1:D:78:LEU:HB3	1:D:92:VAL:HG13	2.01	0.41
1:A:148:LEU:HB3	1:A:510:LEU:HD11	2.03	0.41
1:A:471:ILE:HG12	1:D:128:ILE:HD11	2.03	0.41
1:A:532:ASP:O	1:A:533:ILE:C	2.59	0.41
1:A:95:SER:HA	1:A:519:LEU:HD21	2.03	0.41
1:B:445:GLN:OE1	1:B:449:ARG:NH2	2.53	0.41
1:C:166:ILE:HG13	1:C:409:ILE:HD11	2.03	0.41
1:C:92:VAL:C	1:C:94:LEU:H	2.24	0.41
1:D:225:ILE:HG22	1:D:227:GLY:H	1.85	0.41
1:D:287:GLU:O	1:D:291:GLN:HG2	2.21	0.41
1:B:391:ASN:C	1:B:393:MET:H	2.23	0.41
1:A:126:ARG:HD3	1:D:471:ILE:HD12	2.03	0.41
1:A:194:LEU:O	1:A:197:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:LYS:NZ	1:B:161:ASP:OD2	2.46	0.41
1:B:314:LEU:HG	1:B:319:LEU:HD23	2.03	0.41
1:B:299:LEU:HG	1:B:320:PRO:O	2.20	0.41
1:B:340:ARG:NH1	1:B:353:LEU:HD12	2.33	0.41
1:C:248:ILE:HG12	1:C:299:LEU:HD23	2.02	0.41
1:A:391:ASN:C	1:A:393:MET:H	2.23	0.40
1:B:159:ILE:HG12	1:B:160:LYS:H	1.86	0.40
1:D:408:VAL:HG13	1:D:509:THR:HG21	2.04	0.40
1:D:166:ILE:HG23	1:D:405:ALA:HB1	2.02	0.40
1:C:162:THR:O	1:C:166:ILE:HG12	2.21	0.40
1:C:251:LEU:HD23	1:C:342:VAL:HB	2.03	0.40
1:D:270:SER:O	1:D:272:GLU:N	2.55	0.40
1:D:64:LYS:H	1:D:64:LYS:HD2	1.86	0.40
1:D:340:ARG:HB3	1:D:352:LYS:HA	2.02	0.40
1:B:147:HIS:CD2	1:B:151:ILE:HD11	2.57	0.40
1:B:201:ARG:C	1:B:203:ASP:H	2.25	0.40
1:C:37:HIS:CG	1:C:87:ILE:HG13	2.56	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	486/541 (90%)	413 (85%)	52 (11%)	21 (4%)	2	22
1	B	476/541 (88%)	409 (86%)	52 (11%)	15 (3%)	4	29
1	C	464/541 (86%)	399 (86%)	45 (10%)	20 (4%)	2	22
1	D	439/541 (81%)	370 (84%)	52 (12%)	17 (4%)	3	25
All	All	1865/2164 (86%)	1591 (85%)	201 (11%)	73 (4%)	3	25

All (73) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	MET
1	A	208	LEU
1	A	234	PHE
1	A	392	LYS
1	A	441	PRO
1	A	533	ILE
1	B	320	PRO
1	B	341	ILE
1	B	374	ILE
1	B	441	PRO
1	C	202	ARG
1	C	235	SER
1	C	442	THR
1	C	443	LEU
1	C	530	ILE
1	C	533	ILE
1	D	65	ASP
1	D	93	GLU
1	D	298	ASN
1	A	61	MET
1	A	82	ASP
1	A	199	MET
1	A	509	THR
1	B	72	ASN
1	B	160	LYS
1	B	443	LEU
1	C	346	SER
1	C	392	LYS
1	C	441	PRO
1	C	509	THR
1	C	529	LYS
1	D	296	GLY
1	D	345	PHE
1	D	441	PRO
1	D	509	THR
1	A	59	LYS
1	A	80	MET
1	A	235	SER
1	A	345	PHE
1	B	231	ASP
1	B	236	HIS
1	B	509	THR
1	C	324	TRP

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Mol	Chain	Res	Type
1	D	81	MET
1	D	235	SER
1	D	270	SER
1	A	201	ARG
1	A	231	ASP
1	A	232	LYS
1	A	343	PRO
1	A	396	GLU
1	B	59	LYS
1	B	73	ASP
1	B	232	LYS
1	C	73	ASP
1	C	231	ASP
1	C	236	HIS
1	C	296	GLY
1	C	297	ALA
1	C	304	TRP
1	D	232	LYS
1	D	308	ASP
1	A	374	ILE
1	D	73	ASP
1	D	236	HIS
1	B	392	LYS
1	C	232	LYS
1	D	271	VAL
1	D	343	PRO
1	A	105	GLY
1	C	374	ILE
1	D	374	ILE
1	B	258	PRO

### 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	414/456 (91%)	406 (98%)	8 (2%)	57 80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	407/456 (89%)	402 (99%)	5 (1%)	71	87
1	C	399/456 (88%)	392 (98%)	7 (2%)	59	81
1	D	380/456 (83%)	375 (99%)	5 (1%)	69	86
All	All	1600/1824 (88%)	1575 (98%)	25 (2%)	62	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	PHE
1	A	238	GLN
1	A	285	PHE
1	A	306	PHE
1	A	332	LEU
1	A	344	ARG
1	A	355	PHE
1	A	534	ARG
1	B	99	ASP
1	B	139	GLN
1	B	226	LYS
1	B	259	LYS
1	B	261	LYS
1	C	184	GLN
1	C	205	ASP
1	C	306	PHE
1	C	318	ASN
1	C	372	LEU
1	C	391	ASN
1	C	532	ASP
1	D	34	LEU
1	D	234	PHE
1	D	306	PHE
1	D	348	LEU
1	D	493	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	303	GLN
1	C	311	ASN
1	D	147	HIS

### 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 ⓘ

4 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	B	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.34	4 (13%)
2	ADP	C	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.35	4 (13%)
2	ADP	A	601	-	24,29,29	0.97	1 (4%)	29,45,45	1.35	4 (13%)
2	ADP	D	601	-	24,29,29	0.96	1 (4%)	29,45,45	1.34	4 (13%)

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	B	601	-	-	3/12/32/32	0/3/3/3
2	ADP	C	601	-	-	5/12/32/32	0/3/3/3
2	ADP	A	601	-	-	2/12/32/32	0/3/3/3
2	ADP	D	601	-	-	4/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	ADP	C5-C4	2.51	1.47	1.40
2	D	601	ADP	C5-C4	2.51	1.47	1.40
2	B	601	ADP	C5-C4	2.50	1.47	1.40
2	A	601	ADP	C5-C4	2.47	1.47	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	ADP	N3-C2-N1	-3.26	123.59	128.68
2	C	601	ADP	N3-C2-N1	-3.22	123.65	128.68
2	D	601	ADP	N3-C2-N1	-3.20	123.68	128.68
2	A	601	ADP	N3-C2-N1	-3.20	123.68	128.68
2	A	601	ADP	C3'-C2'-C1'	2.94	105.41	100.98
2	D	601	ADP	C3'-C2'-C1'	2.93	105.39	100.98
2	B	601	ADP	C3'-C2'-C1'	2.88	105.31	100.98
2	C	601	ADP	C4-C5-N7	-2.84	106.44	109.40
2	C	601	ADP	C3'-C2'-C1'	2.84	105.25	100.98
2	D	601	ADP	C4-C5-N7	-2.83	106.45	109.40
2	A	601	ADP	C4-C5-N7	-2.71	106.57	109.40
2	A	601	ADP	PA-O3A-PB	-2.66	123.69	132.83
2	B	601	ADP	C4-C5-N7	-2.66	106.63	109.40
2	B	601	ADP	PA-O3A-PB	-2.58	123.98	132.83
2	C	601	ADP	PA-O3A-PB	-2.44	124.45	132.83
2	D	601	ADP	PA-O3A-PB	-2.32	124.87	132.83

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	ADP	C5'-O5'-PA-O1A
2	C	601	ADP	PB-O3A-PA-O5'
2	A	601	ADP	PB-O3A-PA-O1A
2	B	601	ADP	PB-O3A-PA-O5'
2	D	601	ADP	PB-O3A-PA-O5'
2	C	601	ADP	O4'-C4'-C5'-O5'
2	D	601	ADP	O4'-C4'-C5'-O5'
2	C	601	ADP	C3'-C4'-C5'-O5'
2	A	601	ADP	PB-O3A-PA-O5'
2	D	601	ADP	C3'-C4'-C5'-O5'
2	B	601	ADP	C5'-O5'-PA-O3A
2	C	601	ADP	PB-O3A-PA-O1A

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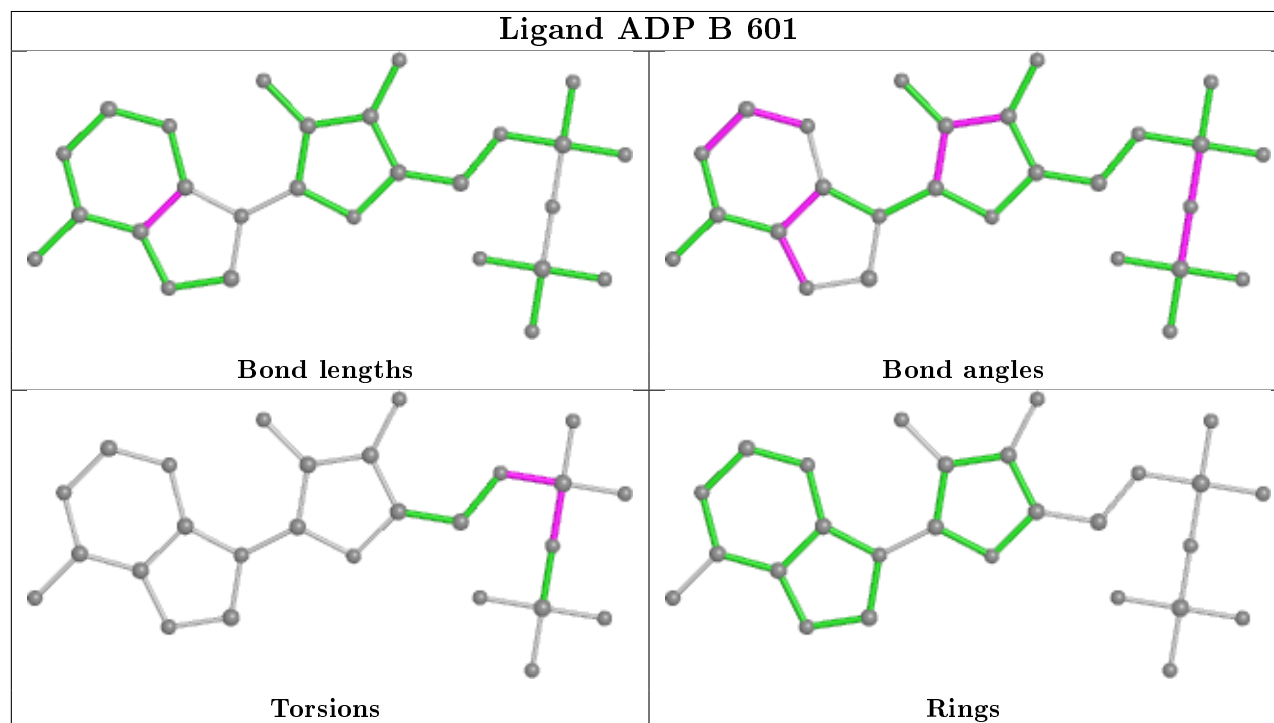
Mol	Chain	Res	Type	Atoms
2	C	601	ADP	PB-O3A-PA-O2A
2	D	601	ADP	PB-O3A-PA-O1A

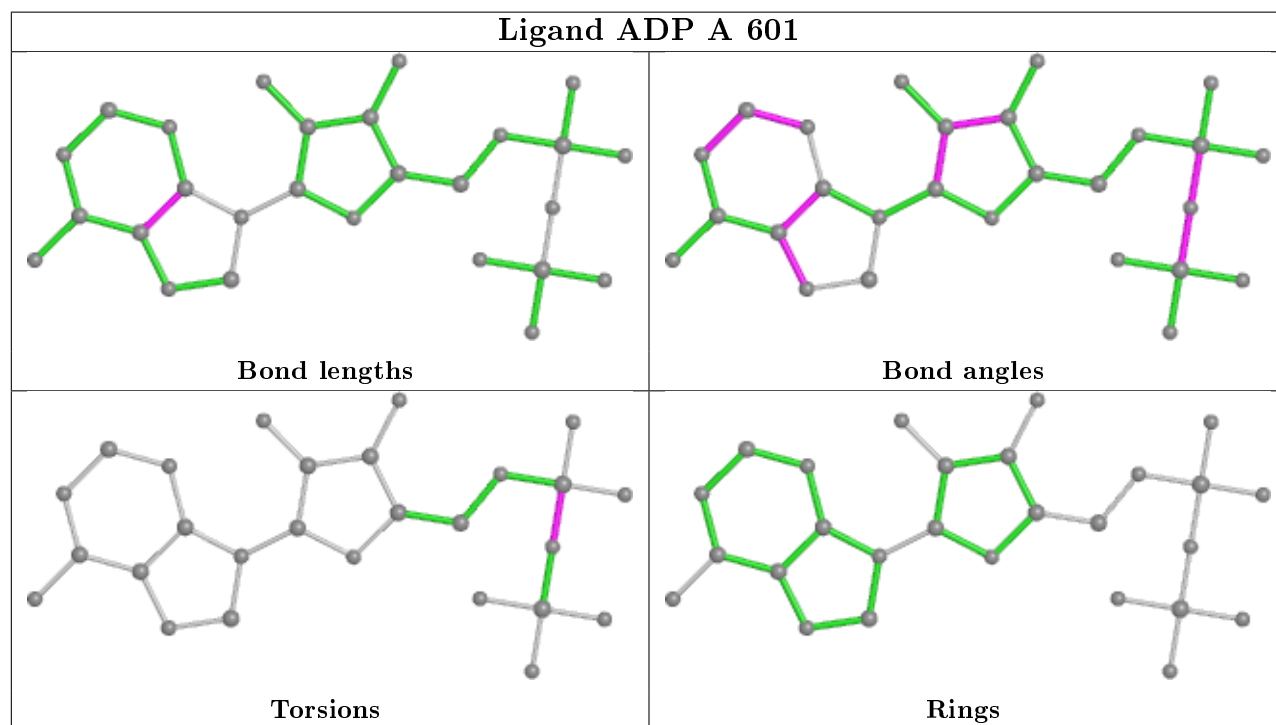
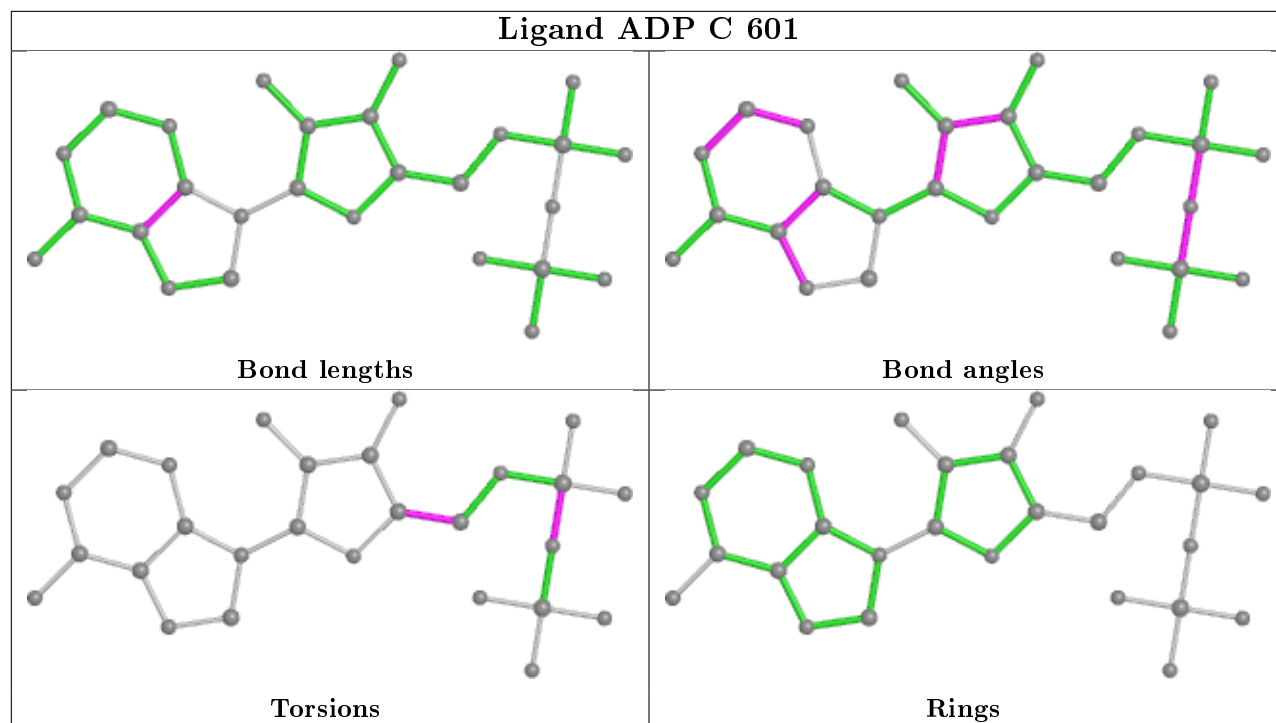
There are no ring outliers.

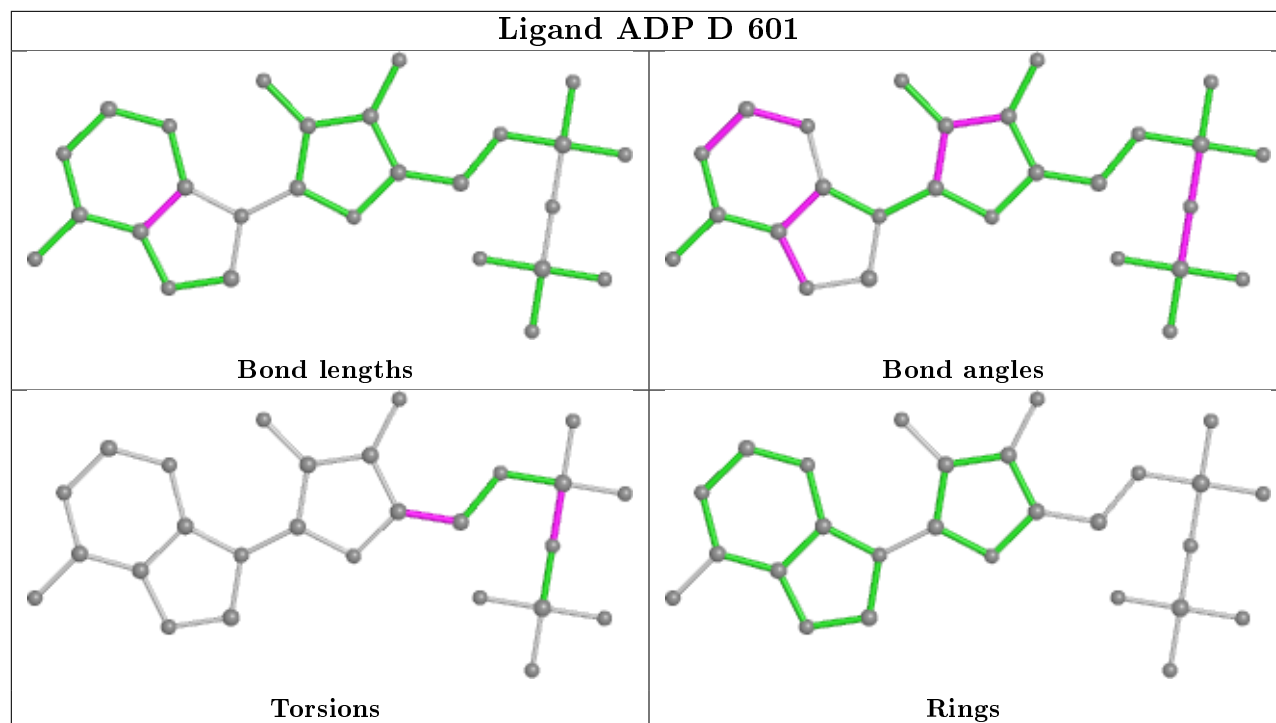
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	ADP	1	0
2	C	601	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, 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	492/541 (90%)	0.27	15 (3%) 50 44	54, 119, 189, 262	0
1	B	484/541 (89%)	0.18	8 (1%) 70 64	48, 102, 167, 269	0
1	C	474/541 (87%)	0.16	14 (2%) 50 44	60, 129, 205, 260	0
1	D	451/541 (83%)	0.28	15 (3%) 46 41	57, 132, 203, 262	0
All	All	1901/2164 (87%)	0.22	52 (2%) 54 48	48, 118, 196, 269	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	SER	5.7
1	A	382	ALA	5.4
1	D	205	ASP	4.4
1	D	370	LYS	4.3
1	A	346	SER	4.2
1	C	370	LYS	4.1
1	C	345	PHE	4.0
1	D	371	MET	3.8
1	C	372	LEU	3.6
1	D	228	VAL	3.4
1	A	391	ASN	3.4
1	A	392	LYS	3.4
1	B	200	GLU	3.2
1	A	199	MET	3.2
1	C	206	PHE	3.1
1	A	385	ILE	3.1
1	D	240	PRO	3.1
1	B	97	SER	2.9
1	C	229	ILE	2.9
1	A	185	MET	2.8
1	D	229	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	248	ILE	2.7
1	C	228	VAL	2.7
1	D	65	ASP	2.7
1	D	306	PHE	2.7
1	A	532	ASP	2.6
1	B	372	LEU	2.6
1	D	95	SER	2.5
1	D	230	VAL	2.5
1	A	228	VAL	2.5
1	C	249	ALA	2.5
1	A	341	ILE	2.4
1	C	348	LEU	2.4
1	B	340	ARG	2.4
1	D	372	LEU	2.4
1	D	307	ASP	2.4
1	C	535	LYS	2.4
1	D	345	PHE	2.4
1	B	337	THR	2.3
1	C	95	SER	2.3
1	C	230	VAL	2.2
1	A	225	ILE	2.2
1	C	534	ARG	2.2
1	D	201	ARG	2.2
1	A	202	ARG	2.2
1	B	98	GLN	2.2
1	C	321	ALA	2.1
1	B	292	ILE	2.1
1	C	532	ASP	2.1
1	A	211	VAL	2.0
1	D	206	PHE	2.0
1	A	229	ILE	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](#)

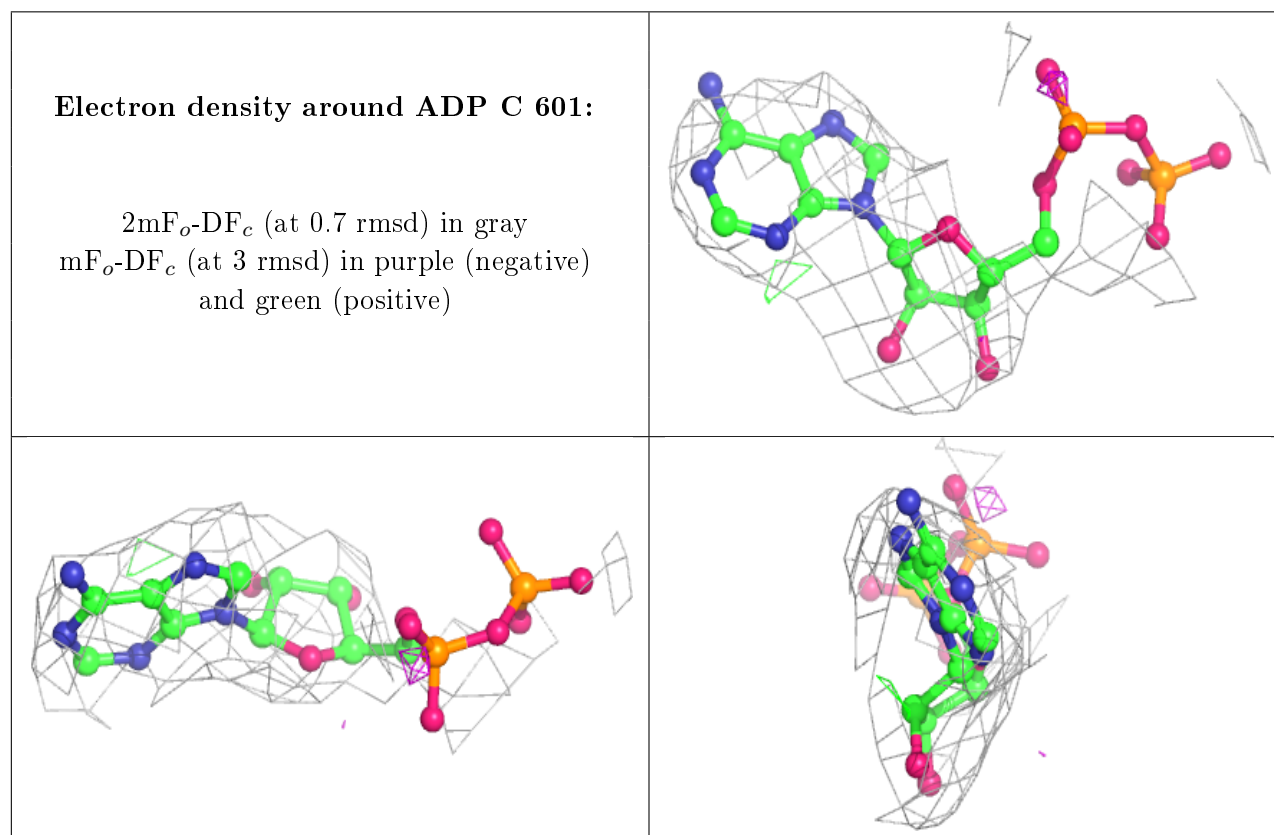
There are no monosaccharides in this entry.

## 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.

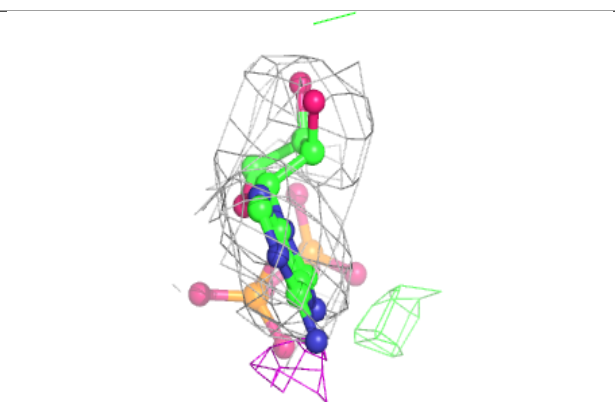
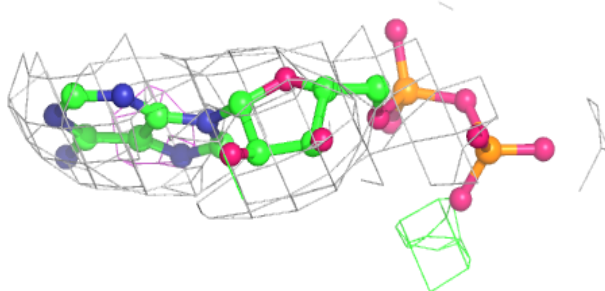
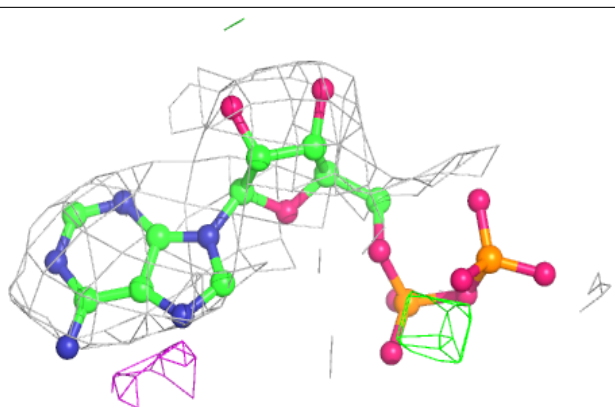
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	C	601	27/27	0.88	0.23	91,94,104,106	0
2	ADP	A	601	27/27	0.89	0.25	76,80,91,92	0
2	ADP	D	601	27/27	0.89	0.26	102,105,112,113	0
2	ADP	B	601	27/27	0.93	0.25	66,68,81,82	0

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.

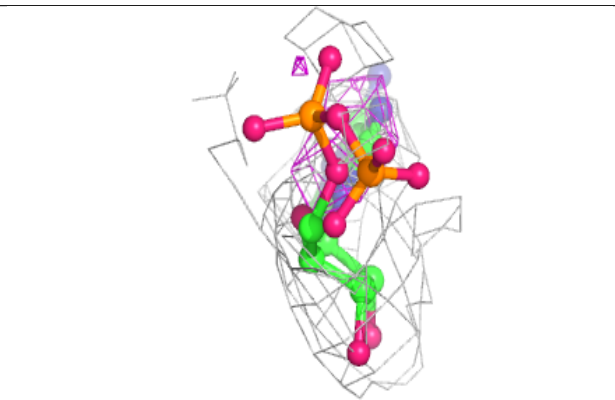
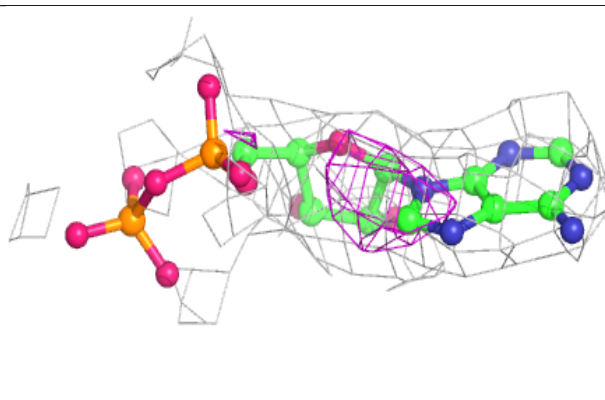
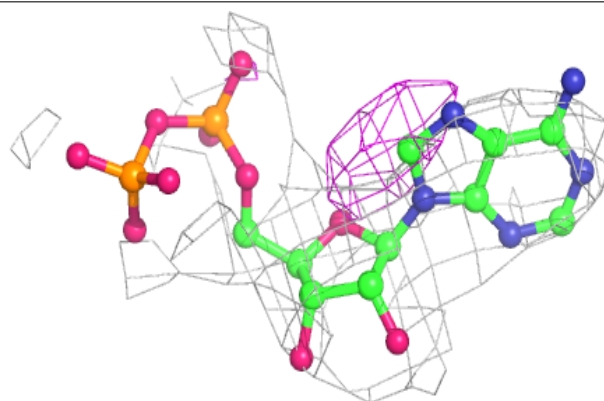


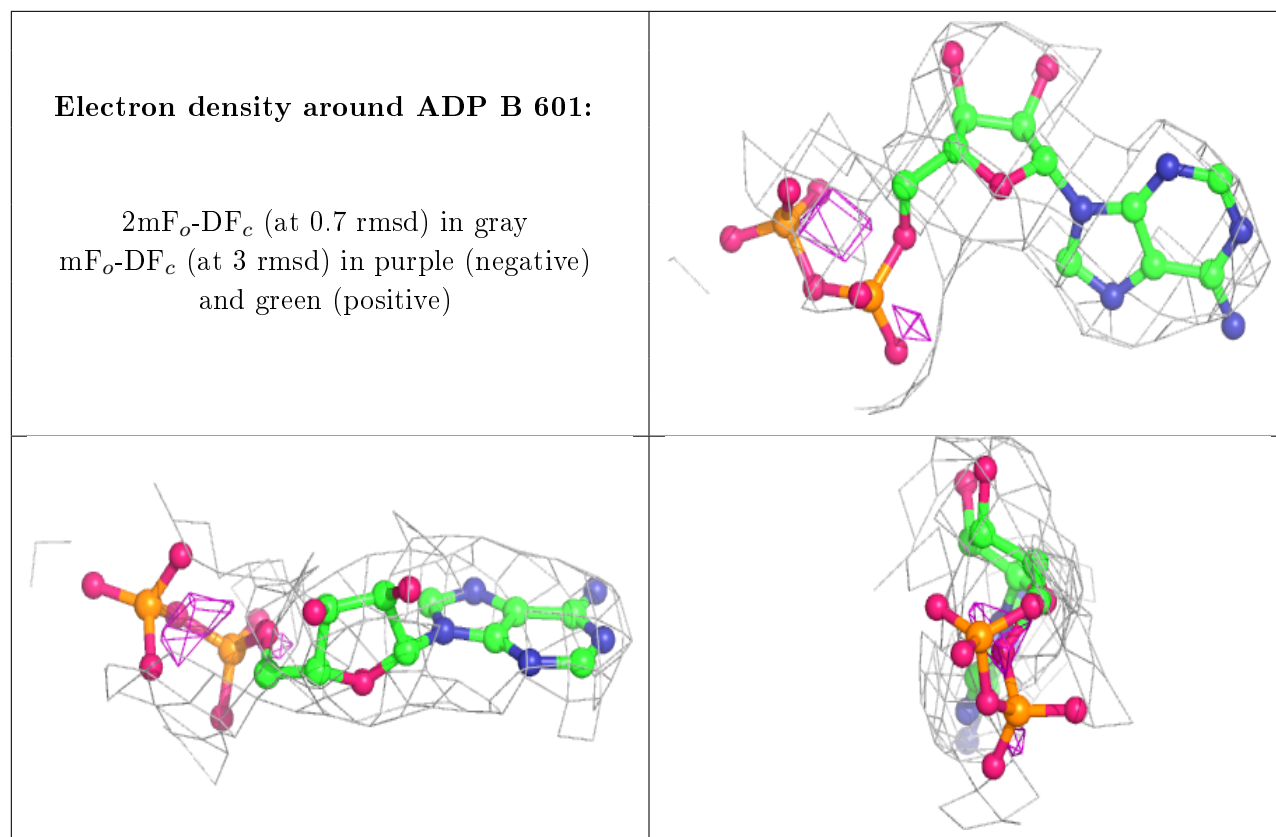
**Electron density around ADP A 601:**

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

**Electron density around ADP D 601:**

$2mF_o-DF_c$  (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.