



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 02:49 PM EDT

PDB ID : 6MFV  
Title : Crystal structure of the Signal Transduction ATPase with Numerous Domains (STAND) protein with a tetratricopeptide repeat sensor PH0952 from *Pyrococcus horikoshii*  
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Deposited on : 2018-09-12  
Resolution : 3.40 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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
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

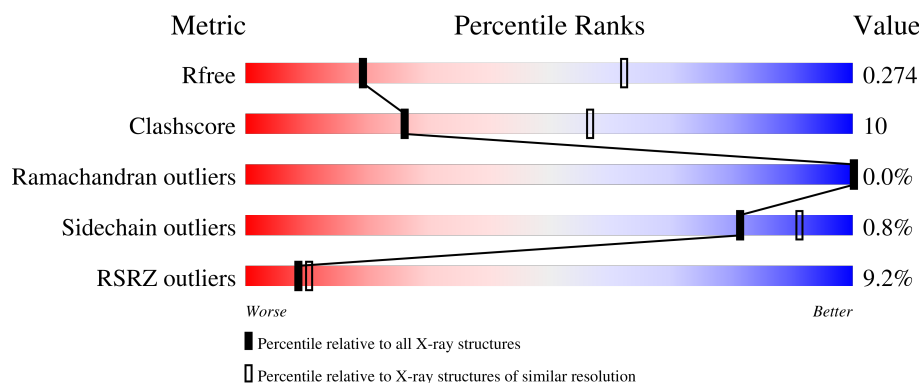
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	653	<div> <div>10%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	653	<div> <div>7%</div> <div> <div></div> <div>70%</div> <div>27%</div> <div>.</div> </div> </div>
1	C	653	<div> <div>13%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	D	653	<div> <div>6%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div>.</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21384 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.

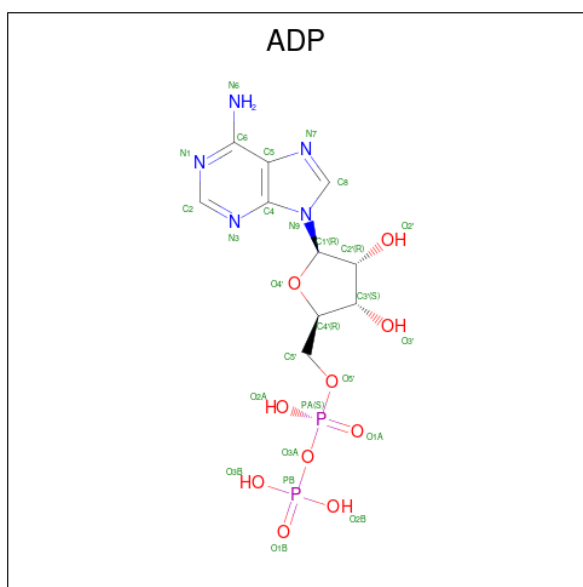
- Molecule 1 is a protein called tetratricopeptide repeat sensor PH0952.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	641	Total	C	N	O	S	0	0	0
			5319	3480	850	973	16			
1	B	641	Total	C	N	O	S	0	0	0
			5319	3480	850	973	16			
1	C	641	Total	C	N	O	S	0	0	0
			5319	3480	850	973	16			
1	D	641	Total	C	N	O	S	0	0	0
			5319	3480	850	973	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MET	-	initiating methionine	UNP O58663
B	101	MET	-	initiating methionine	UNP O58663
C	101	MET	-	initiating methionine	UNP O58663
D	101	MET	-	initiating methionine	UNP O58663

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



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

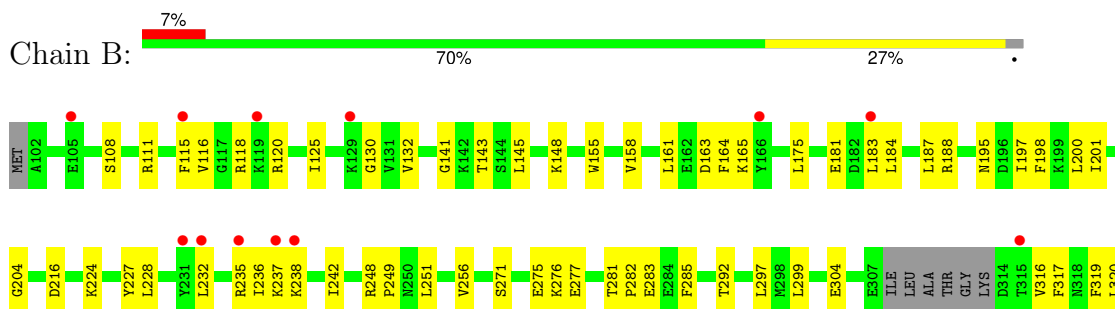
### 3 Residue-property plots

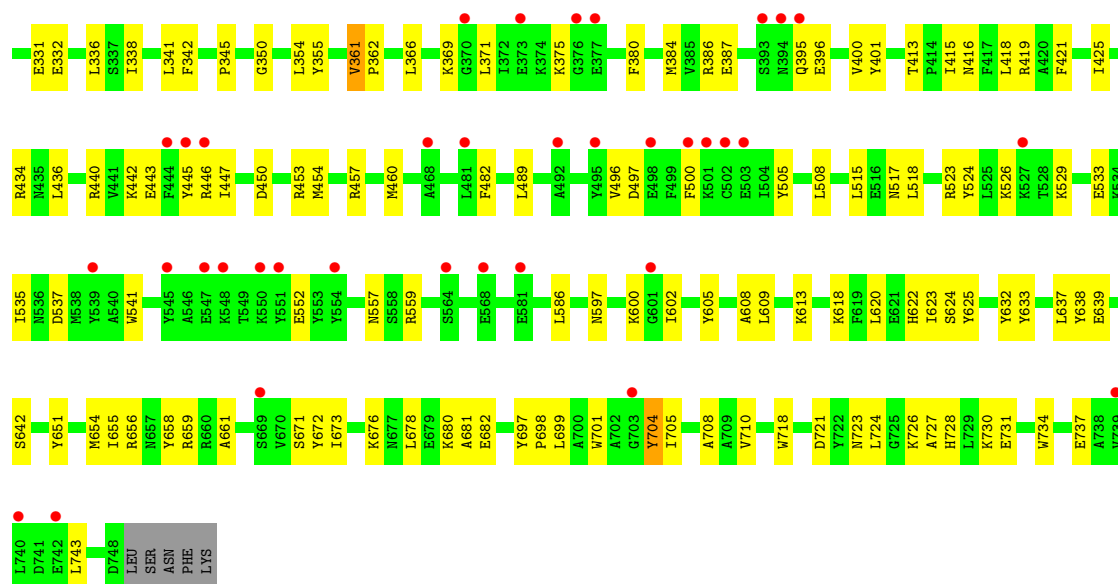
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: tetratricopeptide repeat sensor PH0952

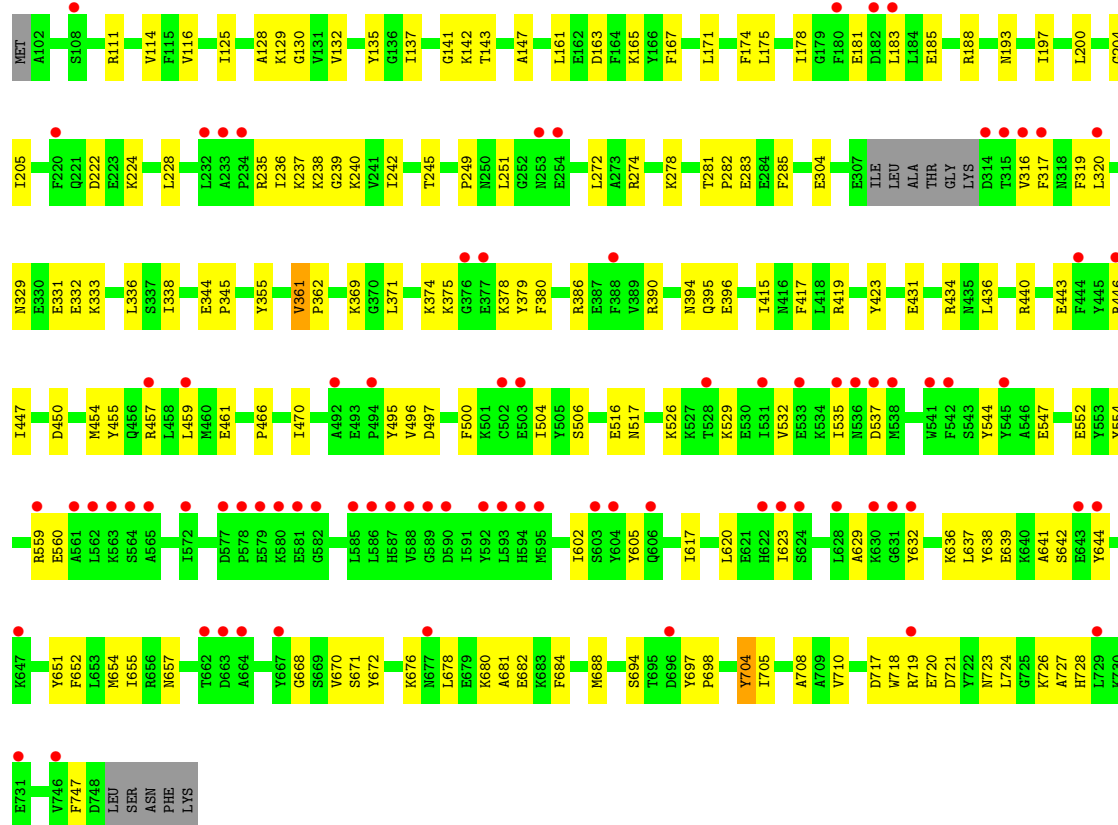
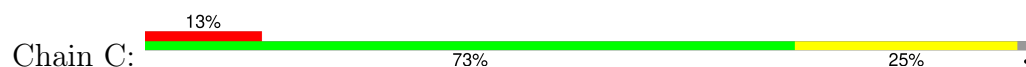


- Molecule 1: tetratricopeptide repeat sensor PH0952



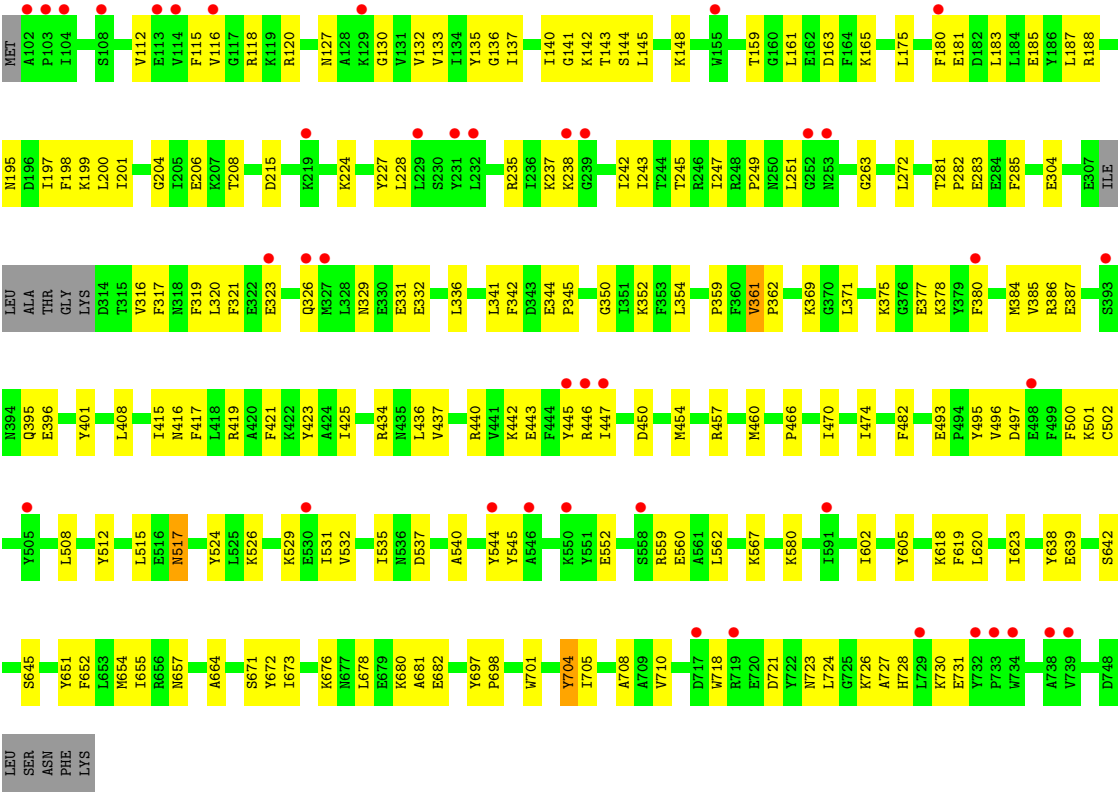


• Molecule 1: tetratricopeptide repeat sensor PH0952



• Molecule 1: tetratricopeptide repeat sensor PH0952





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.13Å 96.13Å 584.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.69 – 3.40 48.69 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.69-3.40) 99.9 (48.69-3.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 3.40Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.224 , 0.272 0.230 , 0.274	Depositor DCC
$R_{free}$ test set	2098 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	104.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 74.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.377 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	21384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	150.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: 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	0/5442	0.38	0/7327
1	B	0.25	0/5442	0.39	0/7327
1	C	0.25	0/5442	0.38	0/7327
1	D	0.25	0/5442	0.39	0/7327
All	All	0.25	0/21768	0.39	0/29308

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	5319	0	5341	105	0
1	B	5319	0	5341	120	0
1	C	5319	0	5341	108	0
1	D	5319	0	5341	122	0
2	A	27	0	12	3	0
2	B	27	0	12	5	0
2	C	27	0	12	4	0
2	D	27	0	12	4	0
All	All	21384	0	21412	443	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 10.

All (443) 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:163:ASP:HB2	1:A:454:MET:HB2	1.66	0.77
1:A:718:TRP:HA	1:A:721:ASP:HB3	1.67	0.76
1:C:336:LEU:HD11	1:C:371:LEU:HD23	1.68	0.76
1:B:708:ALA:HB2	1:B:723:ASN:HB2	1.68	0.75
1:A:222:ASP:OD1	1:D:195:ASN:ND2	2.20	0.74
1:B:163:ASP:HB2	1:B:454:MET:HB2	1.70	0.74
1:D:336:LEU:HD11	1:D:371:LEU:HD23	1.69	0.74
1:D:708:ALA:HB2	1:D:723:ASN:HB2	1.70	0.73
1:A:336:LEU:HD11	1:A:371:LEU:HD23	1.70	0.73
1:D:163:ASP:HB2	1:D:454:MET:HB2	1.70	0.73
1:D:188:ARG:HD3	1:D:200:LEU:HD11	1.70	0.73
1:B:718:TRP:HA	1:B:721:ASP:HB3	1.72	0.72
1:C:708:ALA:HB2	1:C:723:ASN:HB2	1.72	0.71
1:D:682:GLU:HB2	1:D:710:VAL:HG11	1.73	0.70
1:D:345:PRO:HA	1:D:380:PHE:HB3	1.73	0.70
1:D:559:ARG:O	1:D:559:ARG:NH1	2.24	0.70
1:A:275:GLU:O	1:B:523:ARG:NH2	2.25	0.70
1:D:704:TYR:HB3	1:D:727:ALA:HB2	1.74	0.70
1:B:336:LEU:HD11	1:B:371:LEU:HD23	1.73	0.69
1:B:197:ILE:HA	1:B:200:LEU:HD12	1.74	0.69
1:B:345:PRO:HA	1:B:380:PHE:HB3	1.74	0.69
1:B:434:ARG:NH1	1:B:497:ASP:OD2	2.26	0.69
1:B:496:VAL:HB	1:B:500:PHE:HB2	1.74	0.69
1:D:434:ARG:NH1	1:D:497:ASP:OD2	2.26	0.68
1:D:132:VAL:HB	1:D:242:ILE:HG23	1.76	0.68
1:C:163:ASP:HB2	1:C:454:MET:HB2	1.75	0.67
1:C:496:VAL:HB	1:C:500:PHE:HB2	1.76	0.66
1:B:682:GLU:HB2	1:B:710:VAL:HG11	1.77	0.66
1:D:496:VAL:HB	1:D:500:PHE:HB2	1.75	0.66
1:D:175:LEU:HB3	1:D:181:GLU:HB2	1.77	0.66
1:C:175:LEU:HB3	1:C:181:GLU:HB2	1.77	0.65
1:D:446:ARG:HG3	1:D:447:ILE:HG23	1.78	0.65
1:C:345:PRO:HA	1:C:380:PHE:HB3	1.80	0.64
1:D:304:GLU:HG3	1:D:369:LYS:HA	1.80	0.63
1:A:496:VAL:HB	1:A:500:PHE:HB2	1.81	0.63
1:B:704:TYR:HB3	1:B:727:ALA:HB2	1.79	0.63
1:A:345:PRO:HA	1:A:380:PHE:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:ARG:HG3	1:B:447:ILE:HG23	1.81	0.62
1:A:395:GLN:HG2	1:A:396:GLU:HG3	1.80	0.62
1:C:281:THR:HG22	1:C:283:GLU:H	1.65	0.62
1:A:652:PHE:HD2	1:A:657:ASN:HB3	1.63	0.62
1:C:639:GLU:HG3	1:C:676:LYS:HE2	1.82	0.61
1:D:678:LEU:HB3	1:D:710:VAL:HG13	1.83	0.61
1:A:206:GLU:O	1:A:238:LYS:NZ	2.27	0.61
1:D:470:ILE:HD11	1:D:496:VAL:HG11	1.83	0.61
1:A:331:GLU:HG2	1:A:362:PRO:HB3	1.83	0.60
1:D:718:TRP:HA	1:D:721:ASP:HB3	1.82	0.60
1:C:718:TRP:HA	1:C:721:ASP:HB3	1.83	0.60
1:C:446:ARG:HG3	1:C:447:ILE:HG23	1.83	0.60
1:A:281:THR:HG22	1:A:283:GLU:H	1.66	0.60
1:D:130:GLY:H	1:D:235:ARG:NH1	2.00	0.60
1:B:281:THR:HG22	1:B:283:GLU:H	1.65	0.60
1:A:345:PRO:HG2	1:A:375:LYS:HD3	1.83	0.59
1:B:316:VAL:O	1:B:320:LEU:N	2.34	0.59
1:D:316:VAL:O	1:D:320:LEU:N	2.32	0.59
1:C:434:ARG:NH1	1:C:497:ASP:OD2	2.35	0.59
1:A:708:ALA:HB2	1:A:723:ASN:HB2	1.84	0.59
1:D:183:LEU:HB3	1:D:654:MET:SD	2.42	0.59
1:B:183:LEU:HB3	1:B:654:MET:SD	2.42	0.59
1:A:446:ARG:HG3	1:A:447:ILE:HG23	1.84	0.59
1:A:316:VAL:O	1:A:320:LEU:N	2.34	0.59
1:B:175:LEU:HB3	1:B:181:GLU:HB2	1.85	0.59
1:C:137:ILE:O	1:C:142:LYS:NZ	2.28	0.59
1:B:248:ARG:HD3	1:C:694:SER:HB3	1.85	0.58
1:C:682:GLU:HB2	1:C:710:VAL:HG11	1.84	0.58
1:D:281:THR:HG22	1:D:283:GLU:H	1.67	0.58
1:B:345:PRO:HG2	1:B:375:LYS:HD3	1.85	0.58
1:B:132:VAL:HB	1:B:242:ILE:HG23	1.85	0.58
1:A:380:PHE:HD2	1:A:386:ARG:HH22	1.51	0.58
1:B:659:ARG:HH11	1:B:697:TYR:HD1	1.52	0.58
1:B:249:PRO:HB2	1:B:251:LEU:HG	1.85	0.58
1:C:132:VAL:HB	1:C:242:ILE:HG23	1.85	0.58
1:A:132:VAL:HB	1:A:242:ILE:HG23	1.87	0.57
1:C:333:LYS:NZ	1:D:127:ASN:O	2.34	0.57
1:C:197:ILE:HA	1:C:200:LEU:HD12	1.86	0.57
1:C:249:PRO:HB2	1:C:251:LEU:HG	1.87	0.57
1:D:395:GLN:HG2	1:D:396:GLU:HG3	1.86	0.57
1:A:658:TYR:HA	1:A:661:ALA:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LEU:HA	1:D:148:LYS:HE3	1.87	0.56
1:C:128:ALA:O	1:C:240:LYS:NZ	2.38	0.56
1:A:111:ARG:NH2	1:B:518:LEU:H	2.04	0.56
1:C:552:GLU:HG3	1:C:560:GLU:HB3	1.87	0.56
1:C:678:LEU:HB3	1:C:710:VAL:HG13	1.87	0.56
1:D:361:VAL:HG23	1:D:362:PRO:HD3	1.88	0.56
1:D:638:TYR:HB3	1:D:671:SER:O	2.06	0.56
1:D:321:PHE:HZ	1:D:385:VAL:HG13	1.70	0.56
1:B:559:ARG:NH1	1:B:559:ARG:O	2.38	0.55
1:A:175:LEU:HB3	1:A:181:GLU:HB2	1.87	0.55
1:C:431:GLU:OE1	1:C:434:ARG:NE	2.39	0.55
1:B:620:LEU:HD23	1:B:623:ILE:HD12	1.89	0.55
1:A:145:LEU:HA	1:A:148:LYS:HE3	1.88	0.54
1:B:632:TYR:HB3	1:B:637:LEU:HB2	1.89	0.54
1:B:141:GLY:HA2	2:B:801:ADP:H8	1.71	0.54
1:B:331:GLU:HG2	1:B:362:PRO:HB3	1.88	0.54
1:D:673:ILE:HG22	1:D:678:LEU:HA	1.89	0.54
1:B:552:GLU:OE1	1:B:557:ASN:ND2	2.37	0.54
1:C:345:PRO:HB2	1:C:378:LYS:HD3	1.90	0.54
1:B:304:GLU:HG3	1:B:369:LYS:HA	1.88	0.54
1:B:361:VAL:HG23	1:B:362:PRO:HD3	1.89	0.54
1:B:723:ASN:HA	1:B:726:LYS:HB3	1.89	0.54
1:C:652:PHE:HD2	1:C:657:ASN:HB3	1.72	0.54
1:D:415:ILE:HG13	1:D:419:ARG:HE	1.71	0.54
1:A:112:VAL:HG21	2:A:801:ADP:H3'	1.89	0.54
1:A:361:VAL:HG23	1:A:362:PRO:HD3	1.90	0.54
1:D:249:PRO:HB2	1:D:251:LEU:HG	1.89	0.54
1:D:377:GLU:HG2	1:D:378:LYS:HG3	1.90	0.54
1:C:329:ASN:N	1:C:332:GLU:OE1	2.34	0.54
1:A:705:ILE:HG23	1:A:727:ALA:HB3	1.89	0.54
1:C:165:LYS:HD2	1:C:450:ASP:O	2.08	0.54
1:D:345:PRO:HG2	1:D:375:LYS:HD3	1.89	0.54
1:D:136:GLY:HA3	1:D:140:ILE:HG21	1.90	0.53
1:D:165:LYS:HD2	1:D:450:ASP:O	2.08	0.53
1:C:470:ILE:HD11	1:C:496:VAL:HG11	1.90	0.53
1:A:115:PHE:HA	2:A:801:ADP:N1	2.24	0.53
1:A:559:ARG:O	1:A:559:ARG:NH1	2.41	0.53
1:C:559:ARG:O	1:C:559:ARG:NH1	2.41	0.53
1:D:115:PHE:HA	2:D:801:ADP:N1	2.23	0.53
1:B:436:LEU:O	1:B:440:ARG:HG2	2.09	0.53
1:A:168:ALA:O	1:A:172:GLY:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:723:ASN:HA	1:C:726:LYS:HB3	1.91	0.53
1:A:197:ILE:HA	1:A:200:LEU:HD12	1.90	0.53
1:B:609:LEU:HD11	1:B:613:LYS:HE2	1.90	0.53
1:A:316:VAL:HG22	1:A:319:PHE:HB2	1.90	0.52
1:D:651:TYR:O	1:D:655:ILE:HG12	2.09	0.52
1:A:434:ARG:NH1	1:A:497:ASP:OD2	2.42	0.52
1:D:344:GLU:HG2	1:D:419:ARG:NH1	2.25	0.52
1:C:224:LYS:HE3	1:C:228:LEU:HD13	1.91	0.52
1:C:361:VAL:HG23	1:C:362:PRO:HD3	1.92	0.52
1:C:390:ARG:O	1:C:394:ASN:ND2	2.40	0.52
1:B:586:LEU:HD21	1:B:624:SER:HB3	1.91	0.52
1:C:316:VAL:O	1:C:320:LEU:N	2.40	0.52
1:A:141:GLY:HA2	2:A:801:ADP:H8	1.75	0.51
1:B:184:LEU:HG	1:B:654:MET:HG3	1.91	0.51
1:D:130:GLY:H	1:D:235:ARG:HH11	1.57	0.51
1:A:639:GLU:HG3	1:A:676:LYS:HE2	1.90	0.51
1:D:639:GLU:HG3	1:D:676:LYS:HE2	1.93	0.51
1:A:236:ILE:HG22	1:A:239:GLY:H	1.75	0.51
1:B:639:GLU:HG3	1:B:676:LYS:HE2	1.93	0.51
1:B:651:TYR:O	1:B:655:ILE:HG12	2.11	0.51
1:C:395:GLN:HG2	1:C:396:GLU:HG3	1.91	0.51
1:D:181:GLU:HB3	1:D:185:GLU:HB3	1.92	0.51
1:D:197:ILE:HA	1:D:200:LEU:HD12	1.93	0.51
1:D:642:SER:HB2	1:D:672:TYR:HD1	1.76	0.51
1:A:165:LYS:HD2	1:A:450:ASP:O	2.11	0.51
1:B:195:ASN:ND2	1:C:222:ASP:OD1	2.44	0.51
1:C:135:TYR:HA	1:C:245:THR:O	2.11	0.51
1:C:380:PHE:HD2	1:C:386:ARG:HH22	1.59	0.51
1:C:526:LYS:HA	1:C:529:LYS:HE2	1.93	0.51
1:A:390:ARG:O	1:A:394:ASN:ND2	2.37	0.51
1:C:717:ASP:N	1:C:720:GLU:OE1	2.44	0.51
1:B:130:GLY:H	1:B:235:ARG:NH1	2.08	0.50
1:A:642:SER:HB2	1:A:672:TYR:HD1	1.75	0.50
1:B:415:ILE:HG13	1:B:419:ARG:HE	1.76	0.50
1:C:672:TYR:CE2	1:C:680:LYS:HB2	2.46	0.50
1:B:271:SER:O	1:B:275:GLU:N	2.39	0.50
1:B:395:GLN:HG2	1:B:396:GLU:HG3	1.93	0.50
1:B:125:ILE:HG23	1:B:132:VAL:HG11	1.94	0.50
1:D:559:ARG:NH1	1:D:562:LEU:HB2	2.26	0.50
1:A:338:ILE:HG21	1:A:355:TYR:HE1	1.77	0.50
1:C:143:THR:N	2:C:801:ADP:O1A	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:TYR:HB3	1:C:727:ALA:HB2	1.93	0.50
1:C:130:GLY:H	1:C:235:ARG:NH1	2.10	0.50
1:C:602:ILE:HA	1:C:605:TYR:CZ	2.46	0.50
1:D:352:LYS:HG3	1:D:359:PRO:HD3	1.94	0.50
1:D:445:TYR:CE2	1:D:580:LYS:HD3	2.47	0.50
1:D:705:ILE:HG23	1:D:727:ALA:HB3	1.94	0.50
1:B:184:LEU:HD23	1:B:656:ARG:HH22	1.76	0.50
1:B:526:LYS:HA	1:B:529:LYS:HG3	1.94	0.49
1:B:188:ARG:HA	1:B:655:ILE:HG23	1.94	0.49
1:A:214:ILE:HB	1:A:243:ILE:HG22	1.94	0.49
1:D:436:LEU:O	1:D:440:ARG:HG2	2.13	0.49
1:B:145:LEU:HA	1:B:148:LYS:HE3	1.94	0.49
1:A:236:ILE:HG22	1:A:238:LYS:H	1.77	0.49
1:B:116:VAL:H	2:B:801:ADP:HN62	1.59	0.49
1:A:187:LEU:HD11	1:A:618:LYS:HD3	1.94	0.49
1:A:332:GLU:HB3	1:A:366:LEU:HD21	1.95	0.49
1:B:187:LEU:HD13	1:B:651:TYR:HE1	1.77	0.49
1:B:338:ILE:HG21	1:B:355:TYR:HE1	1.76	0.49
1:B:366:LEU:HD22	1:B:371:LEU:HD22	1.93	0.49
1:D:206:GLU:O	1:D:238:LYS:NZ	2.41	0.49
1:C:316:VAL:HG22	1:C:319:PHE:HB2	1.94	0.49
1:C:638:TYR:HB3	1:C:671:SER:O	2.13	0.48
1:D:159:THR:HG21	1:D:419:ARG:HH12	1.77	0.48
1:D:652:PHE:HD1	1:D:657:ASN:HB3	1.78	0.48
1:A:417:PHE:HB3	1:A:440:ARG:NH1	2.28	0.48
1:A:586:LEU:HD21	1:A:624:SER:HB3	1.95	0.48
1:B:350:GLY:O	1:B:354:LEU:HB2	2.13	0.48
1:D:482:PHE:CG	1:D:515:LEU:HD11	2.48	0.48
1:A:659:ARG:HH11	1:A:697:TYR:HD1	1.60	0.48
1:D:457:ARG:HH11	1:D:460:MET:HE3	1.79	0.48
1:A:249:PRO:HB2	1:A:251:LEU:HG	1.94	0.48
1:B:482:PHE:CG	1:B:515:LEU:HD11	2.49	0.48
1:C:116:VAL:HG12	1:C:272:LEU:HD12	1.94	0.48
1:D:645:SER:OG	1:D:664:ALA:O	2.31	0.48
1:B:115:PHE:HA	2:B:801:ADP:N1	2.29	0.48
1:B:705:ILE:HG23	1:B:727:ALA:HB3	1.95	0.48
1:C:304:GLU:HG3	1:C:369:LYS:HA	1.96	0.48
1:A:264:LEU:HG	1:A:296:PRO:HG3	1.95	0.48
1:A:697:TYR:CD1	1:A:698:PRO:HD2	2.50	0.47
1:B:421:PHE:O	1:B:425:ILE:HG12	2.13	0.47
1:D:316:VAL:HG22	1:D:319:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:MET:O	1:D:387:GLU:HG2	2.14	0.47
1:D:701:TRP:CZ2	1:D:730:LYS:HE2	2.49	0.47
1:D:198:PHE:CE1	1:D:227:TYR:HB2	2.49	0.47
1:A:137:ILE:O	1:A:142:LYS:NZ	2.30	0.47
1:C:516:GLU:OE2	1:C:554:TYR:OH	2.31	0.47
1:D:331:GLU:HG2	1:D:362:PRO:HB3	1.96	0.47
1:A:417:PHE:O	1:A:440:ARG:NH2	2.29	0.47
1:A:443:GLU:O	1:A:446:ARG:HG2	2.15	0.47
1:B:108:SER:HA	1:B:155:TRP:CD1	2.50	0.47
1:B:704:TYR:HB3	1:B:727:ALA:CB	2.45	0.47
1:C:188:ARG:HH12	1:C:193:ASN:HA	1.79	0.47
1:C:188:ARG:HD3	1:C:200:LEU:HD11	1.96	0.47
1:C:417:PHE:HB3	1:C:440:ARG:NH1	2.30	0.47
1:C:632:TYR:HB2	1:C:641:ALA:HB2	1.97	0.47
1:A:125:ILE:HG12	1:A:132:VAL:HG11	1.96	0.47
1:A:629:ALA:HB2	1:A:644:TYR:HB2	1.96	0.47
1:C:345:PRO:HG2	1:C:375:LYS:HD3	1.96	0.47
1:C:672:TYR:HB3	1:C:681:ALA:HB2	1.97	0.47
1:D:245:THR:HG22	1:D:247:ILE:H	1.79	0.47
1:C:532:VAL:HG11	1:C:544:TYR:HB2	1.97	0.47
1:C:632:TYR:HB3	1:C:637:LEU:HB2	1.97	0.47
1:D:344:GLU:HG2	1:D:419:ARG:HH11	1.79	0.47
1:B:505:TYR:HB3	1:B:524:TYR:O	2.15	0.46
1:D:723:ASN:HA	1:D:726:LYS:HB3	1.96	0.46
1:A:602:ILE:HA	1:A:605:TYR:CZ	2.50	0.46
1:B:181:GLU:HG3	1:B:204:GLY:HA2	1.97	0.46
1:C:181:GLU:HB3	1:C:185:GLU:HB3	1.98	0.46
1:D:512:TYR:HB3	1:D:517:ASN:HB3	1.97	0.46
1:C:344:GLU:OE1	1:C:423:TYR:OH	2.24	0.46
1:C:705:ILE:HG22	1:C:724:LEU:HA	1.97	0.46
1:A:120:ARG:HA	1:A:120:ARG:HD2	1.81	0.46
1:A:237:LYS:HG3	1:A:238:LYS:HG3	1.97	0.46
1:B:380:PHE:HD2	1:B:386:ARG:HH22	1.62	0.46
1:C:174:PHE:O	1:C:178:ILE:HG12	2.15	0.46
1:A:672:TYR:CE2	1:A:680:LYS:HB2	2.50	0.46
1:B:282:PRO:HA	1:B:285:PHE:CD2	2.51	0.46
1:B:297:LEU:HD23	1:B:384:MET:HE2	1.97	0.46
1:D:532:VAL:HG11	1:D:544:TYR:HB2	1.97	0.46
1:C:236:ILE:HG22	1:C:238:LYS:H	1.81	0.46
1:D:237:LYS:HG3	1:D:238:LYS:HG3	1.98	0.46
1:D:482:PHE:CD1	1:D:515:LEU:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD13	1:A:524:TYR:CE2	2.50	0.46
1:A:620:LEU:HD23	1:A:623:ILE:HD12	1.97	0.46
1:B:602:ILE:HA	1:B:605:TYR:CZ	2.50	0.46
1:C:274:ARG:HB3	1:C:278:LYS:HZ3	1.81	0.46
1:D:181:GLU:HG3	1:D:204:GLY:HA2	1.97	0.46
1:A:183:LEU:HB3	1:A:654:MET:SD	2.56	0.46
1:C:236:ILE:HG22	1:C:239:GLY:H	1.81	0.46
1:A:741:ASP:HA	1:A:744:LYS:HE2	1.97	0.46
1:C:617:ILE:HG22	1:C:620:LEU:H	1.80	0.46
1:A:470:ILE:HD11	1:A:496:VAL:HG11	1.98	0.45
1:A:682:GLU:HB2	1:A:710:VAL:HG11	1.97	0.45
1:C:717:ASP:HB2	1:C:719:ARG:HG2	1.99	0.45
1:D:457:ARG:HA	1:D:457:ARG:HD2	1.77	0.45
1:B:237:LYS:HG3	1:B:238:LYS:HG3	1.97	0.45
1:C:181:GLU:HG3	1:C:204:GLY:HA2	1.98	0.45
1:D:115:PHE:CD2	1:D:148:LYS:HD3	2.51	0.45
1:D:502:CYS:HB2	1:D:531:ILE:HG21	1.98	0.45
1:D:526:LYS:HA	1:D:529:LYS:HE2	1.97	0.45
1:A:408:LEU:HD22	1:A:416:ASN:HD22	1.82	0.45
1:C:116:VAL:H	2:C:801:ADP:HN62	1.63	0.45
1:D:421:PHE:CE1	1:D:425:ILE:HD11	2.52	0.45
1:B:143:THR:N	2:B:801:ADP:O1A	2.49	0.45
1:B:224:LYS:HZ2	1:B:227:TYR:HD2	1.60	0.45
1:A:535:ILE:HG23	1:A:537:ASP:H	1.81	0.45
1:B:228:LEU:HD23	1:B:251:LEU:HD11	1.99	0.45
1:B:622:HIS:HA	1:B:625:TYR:CD2	2.52	0.45
1:C:457:ARG:NH2	1:C:461:GLU:OE1	2.50	0.45
1:D:673:ILE:HG23	1:D:681:ALA:HB3	1.98	0.45
1:A:325:TYR:O	1:A:333:LYS:HE2	2.17	0.45
1:B:535:ILE:HG23	1:B:537:ASP:H	1.82	0.45
1:D:442:LYS:HG2	1:D:443:GLU:HG3	1.98	0.45
1:A:436:LEU:O	1:A:440:ARG:HG2	2.17	0.45
1:B:187:LEU:HD11	1:B:618:LYS:HD3	1.99	0.45
1:D:141:GLY:HA2	2:D:801:ADP:H8	1.82	0.45
1:C:114:VAL:HG13	2:C:801:ADP:H2	1.81	0.44
1:C:141:GLY:HA2	2:C:801:ADP:H8	1.82	0.44
1:D:408:LEU:HD22	1:D:416:ASN:HD22	1.82	0.44
1:D:466:PRO:HG2	1:D:495:TYR:CD2	2.52	0.44
1:A:136:GLY:HA3	1:A:140:ILE:HG21	1.99	0.44
1:A:224:LYS:HE3	1:A:228:LEU:HD13	1.99	0.44
1:B:413:THR:OG1	1:B:416:ASN:OD1	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:642:SER:HB2	1:B:672:TYR:HD1	1.82	0.44
1:B:232:LEU:HD22	1:B:256:VAL:HG22	1.99	0.44
1:A:482:PHE:CG	1:A:515:LEU:HD11	2.52	0.44
1:B:120:ARG:HA	1:B:120:ARG:HD2	1.87	0.44
1:B:673:ILE:HG23	1:B:681:ALA:HB3	1.99	0.44
1:A:115:PHE:CD2	1:A:148:LYS:HD3	2.53	0.44
1:D:323:GLU:O	1:D:326:GLN:HG2	2.18	0.44
1:D:443:GLU:O	1:D:446:ARG:HG2	2.18	0.44
1:B:701:TRP:CZ2	1:B:730:LYS:HE2	2.52	0.44
1:A:272:LEU:HD22	1:A:299:LEU:HD23	2.00	0.44
1:A:482:PHE:CD1	1:A:515:LEU:HD11	2.53	0.44
1:A:717:ASP:HB2	1:A:719:ARG:HG2	2.00	0.44
1:C:436:LEU:O	1:C:440:ARG:HG2	2.18	0.44
1:C:651:TYR:O	1:C:655:ILE:HG12	2.17	0.44
1:D:545:TYR:HE2	1:D:567:LYS:HD3	1.82	0.44
1:B:316:VAL:HG22	1:B:319:PHE:HB2	1.99	0.44
1:D:133:VAL:HG22	1:D:243:ILE:HD11	2.00	0.44
1:C:705:ILE:HG23	1:C:727:ALA:HB3	2.00	0.43
1:D:224:LYS:HE3	1:D:228:LEU:HD13	2.00	0.43
1:D:228:LEU:HD23	1:D:251:LEU:HD11	2.00	0.43
1:D:508:LEU:HD13	1:D:524:TYR:CE2	2.53	0.43
1:A:366:LEU:HD22	1:A:371:LEU:HD22	1.99	0.43
1:B:276:LYS:NZ	1:B:277:GLU:OE2	2.51	0.43
1:C:125:ILE:HG12	1:C:132:VAL:HG11	2.00	0.43
1:C:374:LYS:HD3	1:C:379:TYR:CE2	2.53	0.43
1:D:421:PHE:HB2	1:D:440:ARG:NH2	2.33	0.43
1:B:526:LYS:HA	1:B:529:LYS:HE2	2.00	0.43
1:B:728:HIS:HB3	1:C:317:PHE:CZ	2.53	0.43
1:C:443:GLU:O	1:C:446:ARG:HG2	2.18	0.43
1:D:493:GLU:HG2	1:D:501:LYS:NZ	2.33	0.43
1:D:116:VAL:HG12	1:D:272:LEU:HD12	2.01	0.43
1:D:118:ARG:NH1	1:D:263:GLY:O	2.51	0.43
1:D:434:ARG:O	1:D:437:VAL:HG12	2.18	0.43
1:A:710:VAL:HG12	1:A:714:LYS:HD3	2.00	0.43
1:A:728:HIS:HB3	1:D:317:PHE:CZ	2.54	0.43
1:C:130:GLY:H	1:C:235:ARG:HH11	1.67	0.43
1:C:183:LEU:HB3	1:C:654:MET:SD	2.59	0.43
1:A:118:ARG:H	1:A:118:ARG:HE	1.67	0.43
1:A:704:TYR:HB3	1:A:727:ALA:HB2	2.00	0.43
1:B:701:TRP:HB2	1:B:731:GLU:OE2	2.19	0.43
1:B:731:GLU:HB3	1:B:737:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:619:PHE:CE2	1:D:623:ILE:HD11	2.54	0.43
1:D:705:ILE:HG22	1:D:724:LEU:HA	2.01	0.43
1:A:146:ALA:HB1	1:A:213:ILE:HD13	2.01	0.43
1:B:236:ILE:HG22	1:B:238:LYS:H	1.84	0.43
1:B:317:PHE:HZ	1:C:728:HIS:ND1	2.17	0.43
1:B:533:GLU:HA	1:B:541:TRP:HZ3	1.84	0.43
1:C:668:GLY:O	1:C:672:TYR:HB2	2.18	0.43
1:D:144:SER:OG	2:D:801:ADP:H5'2	2.19	0.43
1:A:163:ASP:HB2	1:A:454:MET:CB	2.44	0.43
1:A:526:LYS:HA	1:A:529:LYS:HE2	2.01	0.43
1:B:605:TYR:HA	1:B:608:ALA:HB3	2.01	0.43
1:C:167:PHE:CZ	1:C:171:LEU:HD22	2.54	0.43
1:C:282:PRO:HA	1:C:285:PHE:CD2	2.54	0.43
1:D:329:ASN:N	1:D:332:GLU:OE1	2.46	0.43
1:A:406:ASN:O	1:A:410:LYS:HG2	2.19	0.42
1:A:431:GLU:O	1:A:435:ASN:ND2	2.52	0.42
1:A:532:VAL:HG11	1:A:544:TYR:HB2	2.01	0.42
1:B:164:PHE:CZ	1:B:198:PHE:HE1	2.36	0.42
1:C:697:TYR:CD1	1:C:698:PRO:HD2	2.54	0.42
1:A:384:MET:O	1:A:387:GLU:HG2	2.19	0.42
1:B:165:LYS:HD2	1:B:450:ASP:O	2.19	0.42
1:B:341:LEU:HB3	1:B:401:TYR:OH	2.19	0.42
1:B:697:TYR:CE2	1:B:699:LEU:HB2	2.54	0.42
1:B:701:TRP:CH2	1:B:730:LYS:HE2	2.54	0.42
1:C:670:VAL:HG13	1:C:747:PHE:CE1	2.54	0.42
1:C:684:PHE:O	1:C:688:MET:HG3	2.19	0.42
1:D:421:PHE:O	1:D:425:ILE:HG12	2.19	0.42
1:D:559:ARG:HH12	1:D:562:LEU:HB2	1.83	0.42
1:A:507:TRP:O	1:A:511:ALA:N	2.50	0.42
1:B:292:THR:HG21	1:B:299:LEU:HA	2.01	0.42
1:B:642:SER:HB2	1:B:672:TYR:CD1	2.55	0.42
1:D:120:ARG:HA	1:D:120:ARG:HD2	1.88	0.42
1:A:338:ILE:HG23	1:A:400:VAL:HG11	2.01	0.42
1:A:726:LYS:HE2	1:D:137:ILE:HG21	2.01	0.42
1:B:342:PHE:CE2	1:B:354:LEU:HD21	2.54	0.42
1:B:633:TYR:OH	1:B:743:LEU:HB3	2.19	0.42
1:B:658:TYR:HA	1:B:661:ALA:HB3	2.01	0.42
1:B:697:TYR:CD1	1:B:698:PRO:HD2	2.54	0.42
1:D:282:PRO:HA	1:D:285:PHE:CD2	2.54	0.42
1:B:130:GLY:H	1:B:235:ARG:HH11	1.66	0.42
1:B:158:VAL:HG22	1:B:216:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:LEU:HD13	1:B:508:LEU:HG	2.02	0.42
1:B:597:ASN:HD21	1:B:600:LYS:NZ	2.18	0.42
1:B:672:TYR:CE2	1:B:680:LYS:HB2	2.55	0.42
1:B:705:ILE:HG22	1:B:724:LEU:HA	2.01	0.42
1:C:125:ILE:HG23	1:C:132:VAL:HG11	2.01	0.42
1:D:697:TYR:CD1	1:D:698:PRO:HD2	2.55	0.42
1:A:684:PHE:O	1:A:688:MET:HG3	2.19	0.42
1:B:197:ILE:O	1:B:201:ILE:HG13	2.19	0.42
1:B:332:GLU:HB3	1:B:366:LEU:HD21	2.02	0.42
1:C:455:TYR:CE2	1:C:459:LEU:HD11	2.55	0.42
1:C:142:LYS:H	1:C:142:LYS:HG2	1.71	0.41
1:C:338:ILE:HG21	1:C:355:TYR:HE1	1.85	0.41
1:C:496:VAL:HG21	1:C:504:ILE:HD12	2.02	0.41
1:A:317:PHE:CZ	1:D:728:HIS:HB3	2.56	0.41
1:D:701:TRP:HB2	1:D:731:GLU:OE2	2.19	0.41
1:A:282:PRO:HA	1:A:285:PHE:CD2	2.55	0.41
1:C:642:SER:HB2	1:C:672:TYR:HD1	1.86	0.41
1:D:142:LYS:H	1:D:142:LYS:HG2	1.59	0.41
1:D:342:PHE:O	1:D:386:ARG:NH2	2.53	0.41
1:C:129:LYS:HA	1:C:235:ARG:CZ	2.50	0.41
1:C:526:LYS:HA	1:C:529:LYS:HG3	2.02	0.41
1:C:636:LYS:HE3	1:C:638:TYR:OH	2.21	0.41
1:D:187:LEU:HD11	1:D:618:LYS:HD3	2.01	0.41
1:B:111:ARG:HD2	1:B:148:LYS:HG2	2.02	0.41
1:C:620:LEU:HD23	1:C:623:ILE:HD12	2.02	0.41
1:D:350:GLY:O	1:D:354:LEU:HB2	2.20	0.41
1:D:470:ILE:O	1:D:474:ILE:HG13	2.20	0.41
1:D:602:ILE:HA	1:D:605:TYR:CZ	2.55	0.41
1:D:620:LEU:HD23	1:D:623:ILE:HD12	2.01	0.41
1:A:668:GLY:O	1:A:672:TYR:HB2	2.21	0.41
1:B:698:PRO:HB3	1:B:734:TRP:CD2	2.56	0.41
1:C:111:ARG:HG2	1:C:147:ALA:HB1	2.03	0.41
1:D:180:PHE:HB2	1:D:208:THR:HG22	2.01	0.41
1:D:552:GLU:HG3	1:D:560:GLU:HB3	2.02	0.41
1:A:341:LEU:HB3	1:A:401:TYR:OH	2.20	0.41
1:A:622:HIS:HA	1:A:625:TYR:CD2	2.55	0.41
1:B:678:LEU:HB3	1:B:710:VAL:HG13	2.03	0.41
1:D:417:PHE:C	1:D:440:ARG:HH12	2.24	0.41
1:D:537:ASP:HB3	1:D:540:ALA:HB3	2.02	0.41
1:A:457:ARG:HA	1:A:457:ARG:HD2	1.85	0.41
1:B:440:ARG:O	1:B:445:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:TYR:HA	1:D:245:THR:O	2.20	0.41
1:A:288:LEU:HD23	1:A:288:LEU:HA	1.95	0.41
1:A:323:GLU:O	1:A:326:GLN:HG2	2.21	0.41
1:A:670:VAL:HG13	1:A:747:PHE:CE1	2.56	0.41
1:B:384:MET:O	1:B:387:GLU:HG2	2.21	0.41
1:B:453:ARG:HD2	1:B:453:ARG:HA	1.93	0.41
1:C:331:GLU:HG2	1:C:362:PRO:HB3	2.02	0.41
1:D:112:VAL:HG21	2:D:801:ADP:H3'	2.03	0.41
1:A:382:HIS:HB3	1:A:385:VAL:HG23	2.03	0.41
1:A:342:PHE:CE1	1:A:354:LEU:HD21	2.56	0.40
1:C:237:LYS:HG3	1:C:238:LYS:HG3	2.02	0.40
1:C:415:ILE:HG13	1:C:419:ARG:HE	1.86	0.40
1:C:466:PRO:HG2	1:C:495:TYR:CD2	2.56	0.40
1:D:199:LYS:HA	1:D:199:LYS:HD3	1.86	0.40
1:D:341:LEU:HB3	1:D:401:TYR:OH	2.21	0.40
1:D:344:GLU:OE1	1:D:423:TYR:OH	2.20	0.40
1:B:418:LEU:HD13	1:B:454:MET:SD	2.61	0.40
1:B:442:LYS:NZ	1:B:443:GLU:OE2	2.54	0.40
1:B:638:TYR:HB3	1:B:671:SER:O	2.20	0.40
1:C:205:ILE:H	1:C:205:ILE:HG12	1.74	0.40
1:D:535:ILE:HG23	1:D:537:ASP:H	1.87	0.40
1:A:140:ILE:HD12	1:A:140:ILE:HA	1.95	0.40
1:A:352:LYS:HG3	1:A:359:PRO:HD3	2.04	0.40
1:B:457:ARG:HA	1:B:457:ARG:HD2	1.94	0.40
1:C:506:SER:HB2	1:C:547:GLU:HG2	2.04	0.40
1:D:143:THR:OG1	1:D:215:ASP:OD1	2.37	0.40
1:D:197:ILE:O	1:D:201:ILE:HG13	2.21	0.40
1:B:143:THR:OG1	2:B:801:ADP:O1B	2.34	0.40
1:B:248:ARG:HB2	1:C:694:SER:HA	2.03	0.40
1:B:338:ILE:HG23	1:B:400:VAL:HG11	2.03	0.40
1:C:535:ILE:HG23	1:C:537:ASP:H	1.86	0.40
1:C:629:ALA:HB2	1:C:644:TYR:HB2	2.03	0.40
1:A:248:ARG:HA	1:A:249:PRO:HD3	1.97	0.40
1:A:434:ARG:O	1:A:437:VAL:HG12	2.21	0.40
1:B:457:ARG:HH11	1:B:460:MET:HE3	1.85	0.40
1:C:111:ARG:HD3	1:C:147:ALA:C	2.42	0.40
1:D:672:TYR:CE2	1:D:680:LYS:HB2	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	637/653 (98%)	611 (96%)	25 (4%)	1 (0%)	47	78
1	B	637/653 (98%)	612 (96%)	25 (4%)	0	100	100
1	C	637/653 (98%)	611 (96%)	26 (4%)	0	100	100
1	D	637/653 (98%)	611 (96%)	26 (4%)	0	100	100
All	All	2548/2612 (98%)	2445 (96%)	102 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	ILE

### 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	561/571 (98%)	556 (99%)	5 (1%)	78	90
1	B	561/571 (98%)	556 (99%)	5 (1%)	78	90
1	C	561/571 (98%)	557 (99%)	4 (1%)	84	92
1	D	561/571 (98%)	557 (99%)	4 (1%)	84	92
All	All	2244/2284 (98%)	2226 (99%)	18 (1%)	81	91

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	161	LEU
1	A	361	VAL
1	A	517	ASN
1	A	704	TYR
1	B	118	ARG
1	B	161	LEU
1	B	361	VAL
1	B	517	ASN
1	B	704	TYR
1	C	161	LEU
1	C	361	VAL
1	C	517	ASN
1	C	704	TYR
1	D	161	LEU
1	D	361	VAL
1	D	517	ASN
1	D	704	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	A	801	-	24,29,29	0.67	0	29,45,45	0.66	1 (3%)
2	ADP	B	801	-	24,29,29	0.70	0	29,45,45	0.76	1 (3%)
2	ADP	D	801	-	24,29,29	0.77	0	29,45,45	0.91	2 (6%)
2	ADP	C	801	-	24,29,29	0.80	0	29,45,45	0.90	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
2	ADP	A	801	-	-	4/12/32/32	0/3/3/3
2	ADP	B	801	-	-	0/12/32/32	0/3/3/3
2	ADP	D	801	-	-	2/12/32/32	0/3/3/3
2	ADP	C	801	-	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ADP	C5-C6-N6	2.36	123.90	120.31
2	A	801	ADP	C5-C6-N6	2.27	123.77	120.31
2	C	801	ADP	C5-C6-N6	2.25	123.74	120.31
2	B	801	ADP	C5-C6-N6	2.21	123.68	120.31
2	D	801	ADP	O2B-PB-O3A	2.09	111.64	104.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ADP	PA-O3A-PB-O1B
2	A	801	ADP	C5'-O5'-PA-O1A
2	A	801	ADP	PA-O3A-PB-O2B
2	A	801	ADP	PA-O3A-PB-O3B
2	D	801	ADP	PB-O3A-PA-O1A

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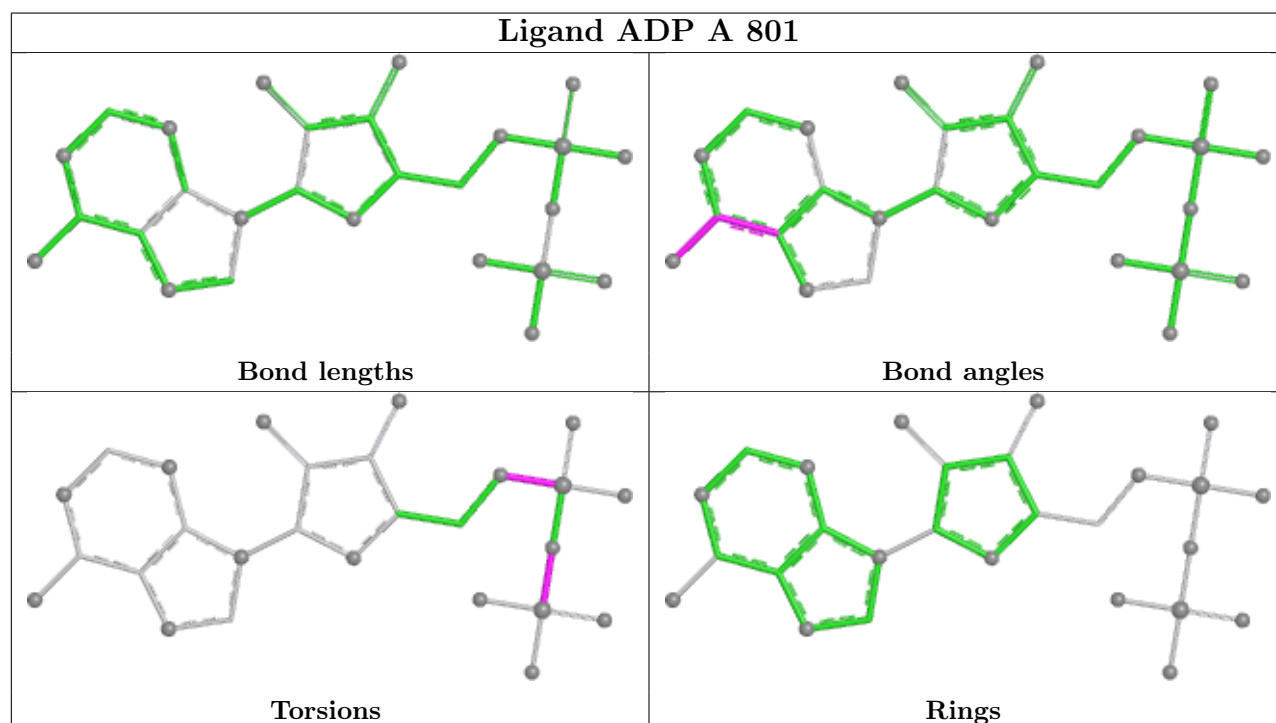
Mol	Chain	Res	Type	Atoms
2	D	801	ADP	PB-O3A-PA-O2A

There are no ring outliers.

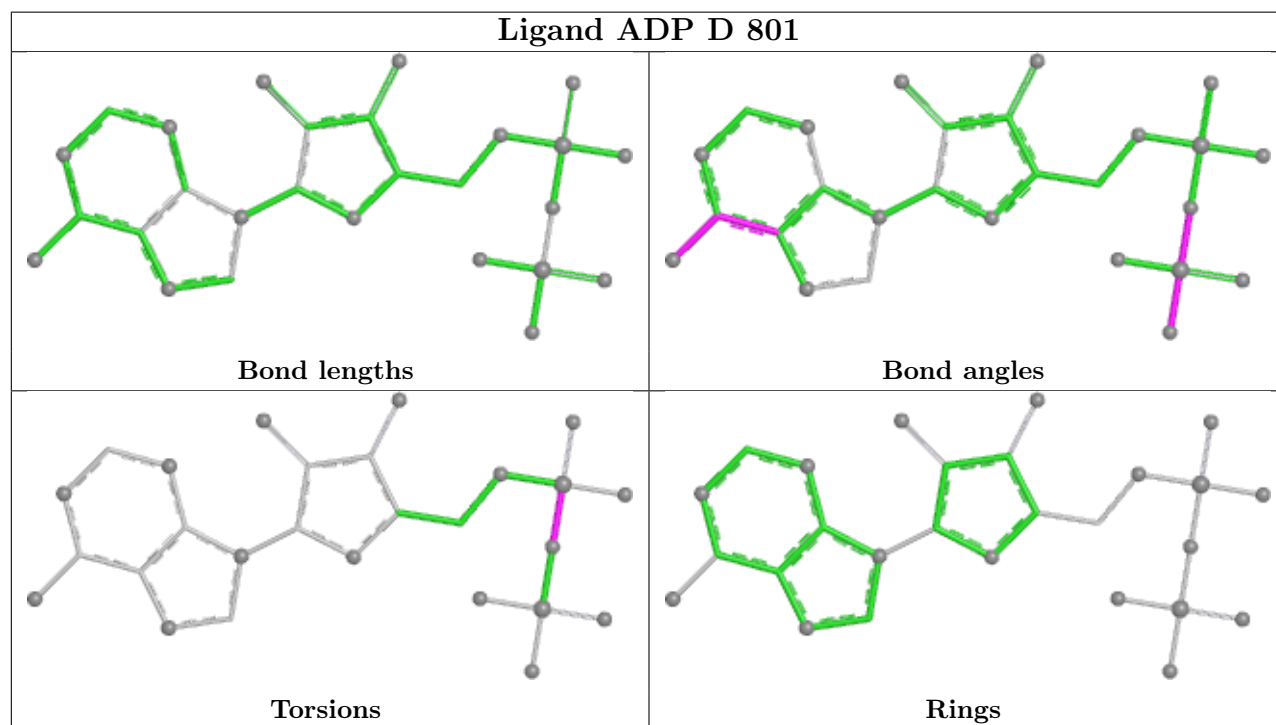
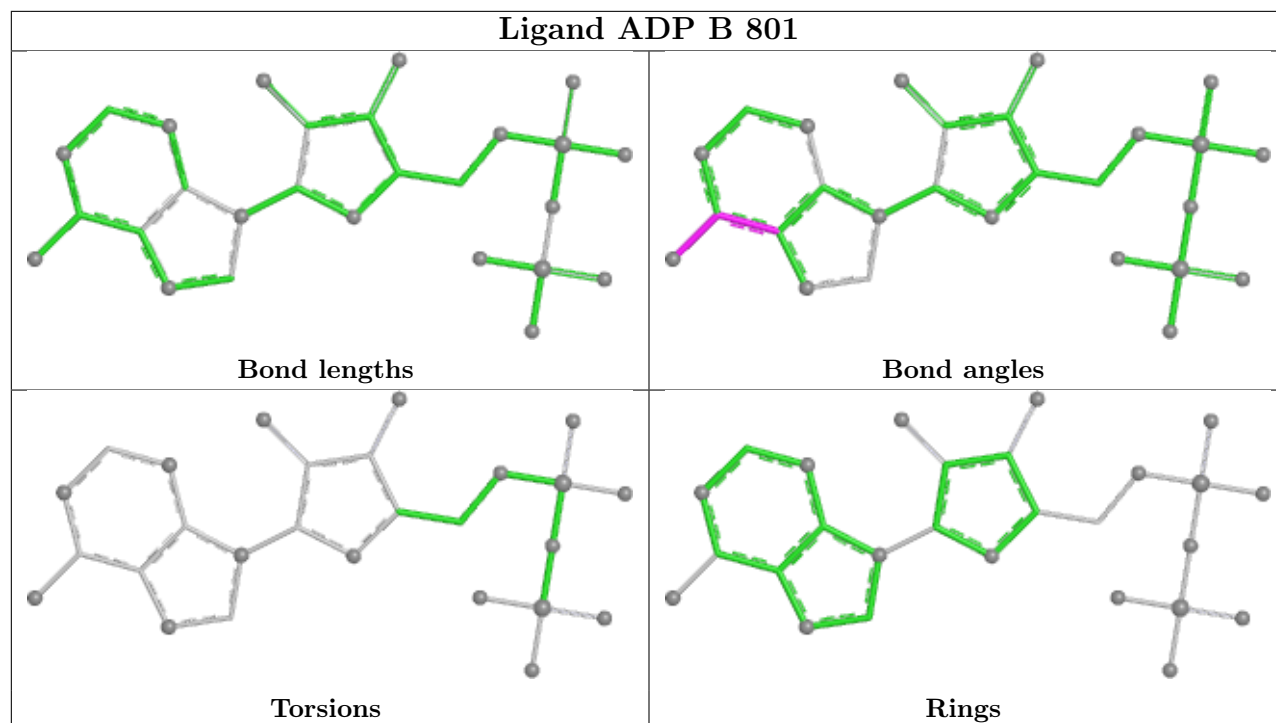
4 monomers are involved in 16 short contacts:

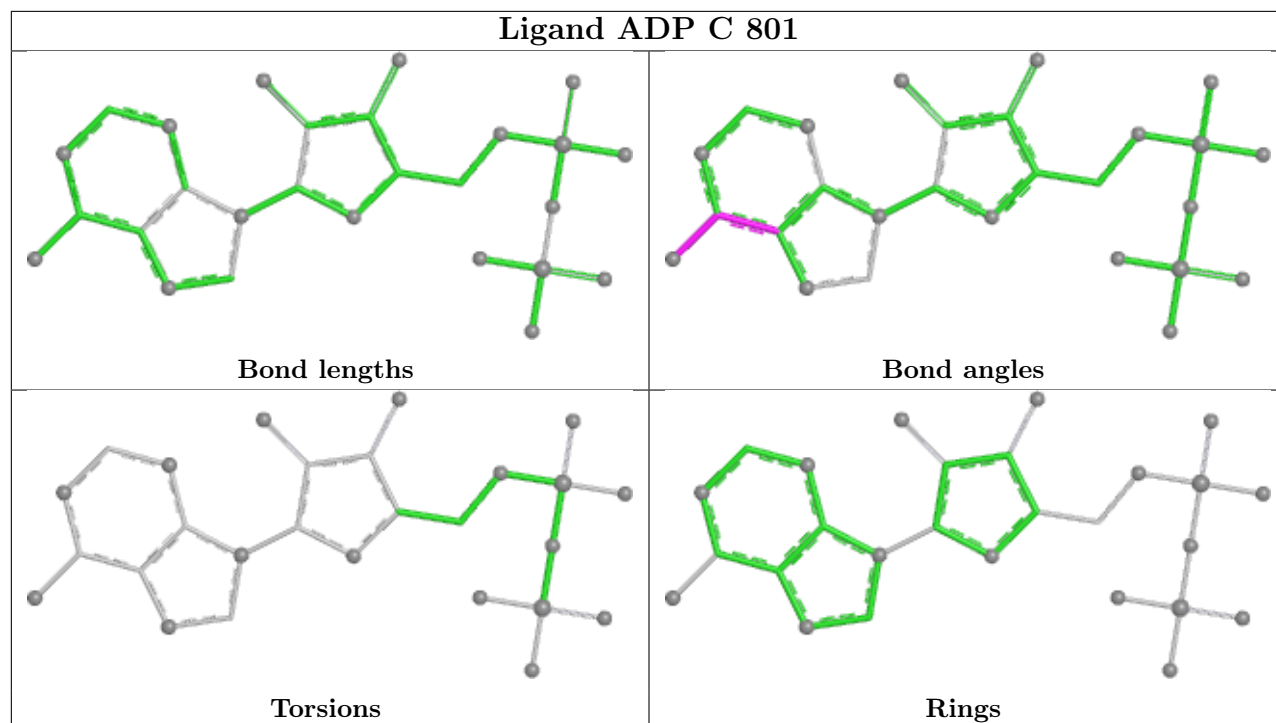
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	ADP	3	0
2	B	801	ADP	5	0
2	D	801	ADP	4	0
2	C	801	ADP	4	0

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	641/653 (98%)	0.39	64 (9%) <b>7</b> <b>8</b>	72, 153, 268, 414	0
1	B	641/653 (98%)	0.17	48 (7%) <b>14</b> <b>16</b>	59, 118, 241, 480	0
1	C	641/653 (98%)	0.49	82 (12%) <b>3</b> <b>4</b>	69, 148, 303, 536	0
1	D	641/653 (98%)	0.08	42 (6%) <b>18</b> <b>20</b>	55, 119, 227, 392	0
All	All	2564/2612 (98%)	0.28	236 (9%) <b>9</b> <b>10</b>	55, 134, 266, 536	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	102	ALA	15.4
1	C	315	THR	11.9
1	D	103	PRO	11.2
1	D	252	GLY	9.3
1	A	545	TYR	9.0
1	C	594	HIS	8.7
1	C	587	HIS	8.6
1	B	394	ASN	8.3
1	D	108	SER	8.2
1	A	596	GLY	8.1
1	C	586	LEU	7.9
1	A	597	ASN	7.9
1	C	593	LEU	7.8
1	C	588	VAL	7.7
1	D	253	ASN	7.6
1	A	110	PRO	7.4
1	C	537	ASP	7.3
1	C	502	CYS	7.3
1	B	551	TYR	7.1
1	A	492	ALA	7.1
1	C	563	LYS	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	592	TYR	7.0
1	B	232	LEU	6.8
1	C	579	GLU	6.7
1	A	562	LEU	6.6
1	A	539	TYR	6.5
1	C	564	SER	6.4
1	C	585	LEU	6.4
1	C	180	PHE	6.2
1	C	446	ARG	6.2
1	C	643	GLU	6.1
1	B	601	GLY	5.8
1	C	377	GLU	5.7
1	C	562	LEU	5.7
1	B	231	TYR	5.6
1	A	667	TYR	5.6
1	A	315	THR	5.4
1	C	580	LYS	5.4
1	A	593	LEU	5.4
1	A	570	GLU	5.3
1	A	599	GLU	5.3
1	A	594	HIS	5.2
1	A	724	LEU	5.2
1	B	237	LYS	5.1
1	C	644	TYR	4.9
1	A	598	TYR	4.9
1	A	728	HIS	4.9
1	A	628	LEU	4.8
1	B	492	ALA	4.8
1	B	501	LYS	4.8
1	C	541	TRP	4.8
1	A	587	HIS	4.8
1	A	186	TYR	4.8
1	D	229	LEU	4.7
1	C	631	GLY	4.6
1	A	645	SER	4.5
1	D	116	VAL	4.5
1	A	502	CYS	4.5
1	C	623	ILE	4.4
1	A	210	ALA	4.3
1	B	315	THR	4.3
1	C	577	ASP	4.3
1	A	590	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	668	GLY	4.1
1	A	394	ASN	4.1
1	B	235	ARG	4.1
1	D	558	SER	4.0
1	B	444	PHE	4.0
1	D	327	MET	4.0
1	B	539	TYR	4.0
1	B	547	GLU	4.0
1	C	582	GLY	4.0
1	C	559	ARG	3.9
1	B	739	VAL	3.9
1	B	554	TYR	3.8
1	C	234	PRO	3.8
1	A	669	SER	3.8
1	C	320	LEU	3.8
1	C	590	ASP	3.8
1	C	538	MET	3.8
1	A	664	ALA	3.8
1	C	542	PHE	3.8
1	A	318	ASN	3.7
1	C	595	MET	3.7
1	A	634	GLN	3.7
1	C	316	VAL	3.7
1	C	630	LYS	3.7
1	B	395	GLN	3.7
1	B	129	LYS	3.6
1	B	373	GLU	3.6
1	A	529	LYS	3.6
1	C	317	PHE	3.6
1	B	550	LYS	3.5
1	C	624	SER	3.5
1	D	739	VAL	3.5
1	C	533	GLU	3.5
1	C	528	THR	3.5
1	B	503	GLU	3.4
1	B	581	GLU	3.4
1	C	664	ALA	3.5
1	A	285	PHE	3.4
1	D	734	TRP	3.4
1	D	180	PHE	3.4
1	A	208	THR	3.4
1	C	108	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	104	ILE	3.2
1	A	630	LYS	3.2
1	C	492	ALA	3.2
1	C	545	TYR	3.2
1	D	530	GLU	3.2
1	B	119	LYS	3.2
1	D	447	ILE	3.2
1	D	498	GLU	3.1
1	B	393	SER	3.1
1	C	531	ILE	3.1
1	A	588	VAL	3.1
1	D	544	TYR	3.1
1	A	573	ARG	3.1
1	C	561	ALA	3.1
1	B	495	TYR	3.0
1	B	548	LYS	3.0
1	D	445	TYR	3.0
1	C	589	GLY	3.0
1	C	578	PRO	3.0
1	A	180	PHE	2.9
1	A	380	PHE	2.9
1	B	564	SER	2.9
1	A	563	LYS	2.9
1	B	370	GLY	2.9
1	A	589	GLY	2.8
1	C	314	ASP	2.8
1	C	572	ILE	2.8
1	D	550	LYS	2.8
1	B	742	GLU	2.8
1	A	453	ARG	2.8
1	A	279	SER	2.8
1	C	494	PRO	2.8
1	B	669	SER	2.8
1	A	572	ILE	2.8
1	B	446	ARG	2.8
1	C	628	LEU	2.8
1	C	662	THR	2.8
1	C	746	VAL	2.7
1	D	732	TYR	2.7
1	A	558	SER	2.7
1	C	677	ASN	2.7
1	B	468	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	359	PRO	2.7
1	A	387	GLU	2.7
1	B	445	TYR	2.7
1	A	501	LYS	2.7
1	D	733	PRO	2.6
1	D	393	SER	2.6
1	D	446	ARG	2.6
1	A	571	ILE	2.6
1	B	500	PHE	2.6
1	C	220	PHE	2.6
1	D	505	TYR	2.6
1	A	671	SER	2.6
1	A	444	PHE	2.6
1	C	232	LEU	2.6
1	D	729	LEU	2.6
1	C	647	LYS	2.5
1	A	663	ASP	2.5
1	C	731	GLU	2.5
1	C	376	GLY	2.5
1	C	182	ASP	2.5
1	D	238	LYS	2.5
1	C	503	GLU	2.5
1	D	591	ILE	2.5
1	D	232	LEU	2.5
1	C	696	ASP	2.5
1	D	717	ASP	2.5
1	C	622	HIS	2.5
1	A	237	LYS	2.4
1	A	592	TYR	2.4
1	C	253	ASN	2.4
1	A	109	SER	2.4
1	B	377	GLU	2.4
1	C	457	ARG	2.4
1	A	461	GLU	2.4
1	B	115	PHE	2.4
1	A	317	PHE	2.4
1	A	586	LEU	2.4
1	B	740	LEU	2.4
1	D	239	GLY	2.3
1	D	380	PHE	2.3
1	C	604	TYR	2.3
1	C	536	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	114	VAL	2.3
1	C	459	LEU	2.3
1	D	738	ALA	2.3
1	D	219	LYS	2.3
1	B	183	LEU	2.3
1	C	663	ASP	2.3
1	C	565	ALA	2.3
1	D	155	TRP	2.3
1	D	129	LYS	2.3
1	D	719	ARG	2.3
1	B	238	LYS	2.3
1	C	603	SER	2.3
1	C	581	GLU	2.2
1	A	425	ILE	2.2
1	C	632	TYR	2.2
1	D	113	GLU	2.2
1	C	444	PHE	2.2
1	C	535	ILE	2.2
1	B	527	LYS	2.2
1	D	326	GLN	2.2
1	B	166	TYR	2.2
1	B	502	CYS	2.2
1	C	254	GLU	2.1
1	D	323	GLU	2.1
1	A	404	HIS	2.1
1	A	733	PRO	2.1
1	D	231	TYR	2.1
1	A	530	GLU	2.1
1	C	729	LEU	2.1
1	B	545	TYR	2.1
1	B	568	GLU	2.1
1	D	546	ALA	2.1
1	A	559	ARG	2.1
1	C	388	PHE	2.1
1	A	604	TYR	2.1
1	B	498	GLU	2.1
1	C	667	TYR	2.1
1	C	606	GLN	2.1
1	A	647	LYS	2.0
1	B	376	GLY	2.0
1	B	703	GLY	2.0
1	A	323	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	183	LEU	2.0
1	C	233	ALA	2.0
1	C	719	ARG	2.0
1	B	105	GLU	2.0
1	B	481	LEU	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](#)

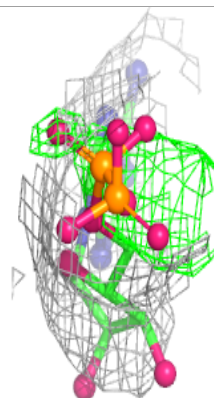
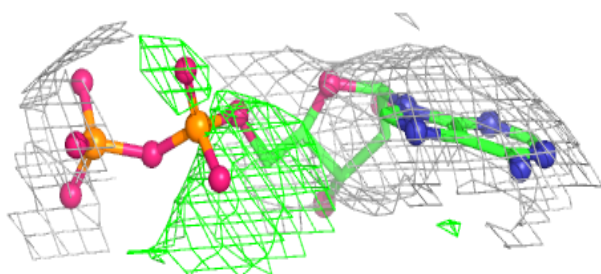
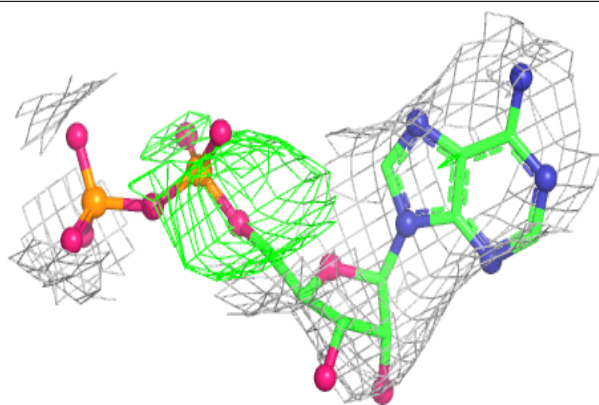
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	D	801	27/27	0.91	0.26	70,130,180,190	0
2	ADP	B	801	27/27	0.95	0.20	0,96,125,136	0
2	ADP	C	801	27/27	0.96	0.17	22,105,139,151	0
2	ADP	A	801	27/27	0.97	0.16	24,85,124,129	0

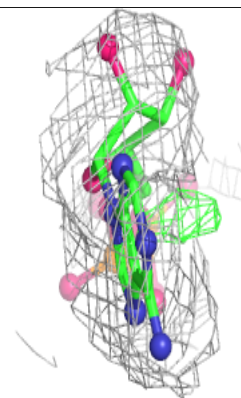
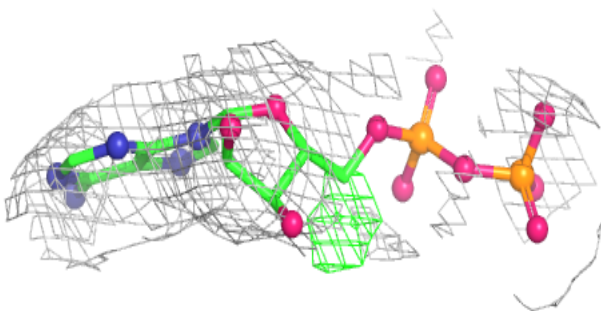
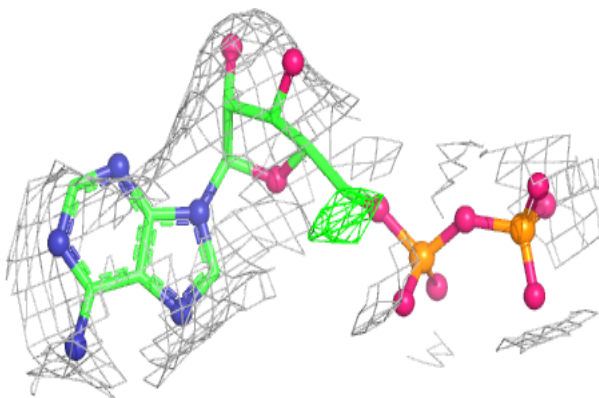
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around ADP D 801:**

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

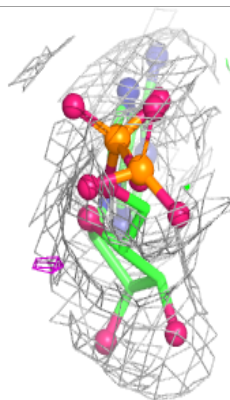
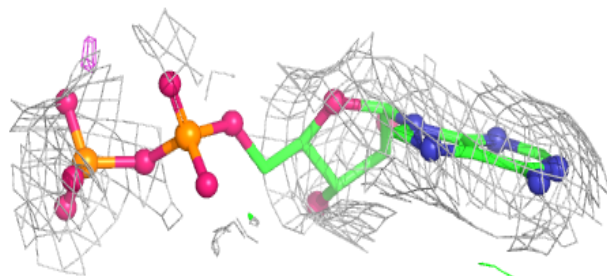
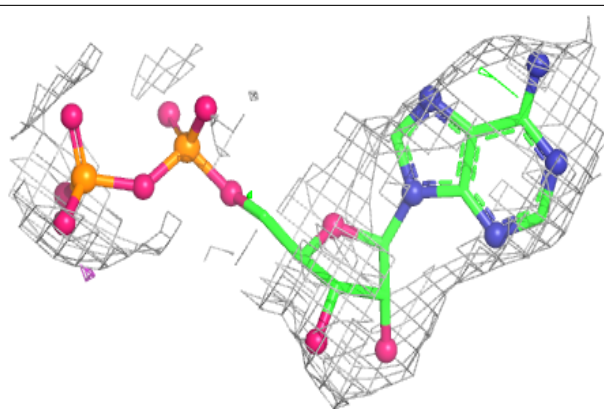
**Electron density around ADP B 801:**

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

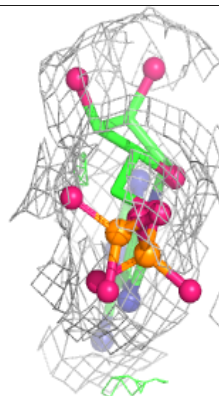
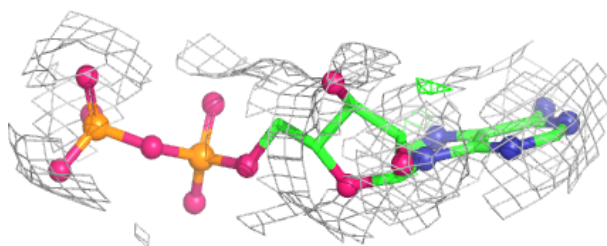
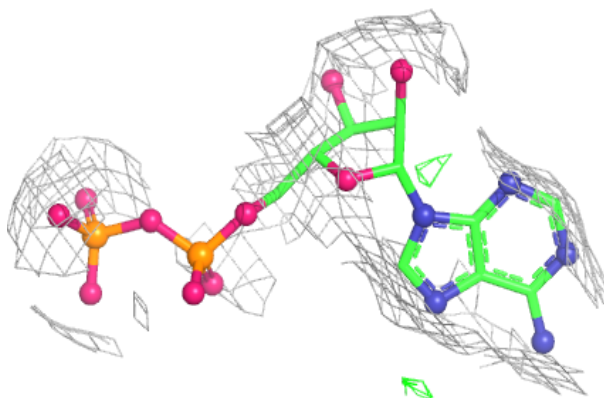


**Electron density around ADP C 801:**

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

**Electron density around ADP A 801:**

$2mF_o - DF_c$  (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.