Full wwPDB X-ray Structure Validation Report (i)

Sep 18, 2023 – 05:22 PM EDT

PDB ID	:	5BU2
Title	:	Structure of the C-terminal domain of lpg1496 from Legionella pneumophila in complex with nucleotide
Authors	:	Wong, K.; Kozlov, G.; Gehring, K.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on	:	2015-06-03
Resolution	:	2.11 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

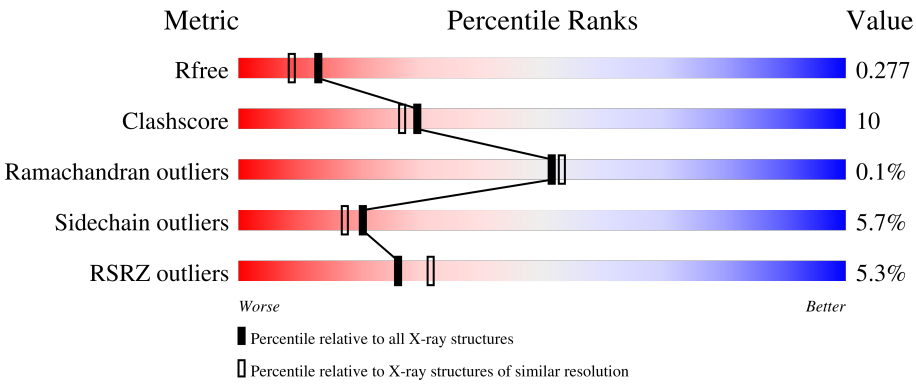
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	454	4% 49% 13% • 37%
1	B	454	2% 51% 12% • 36%
1	C	454	2% 52% 11% • 36%
1	D	454	6% 50% 12% • 36%

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
2	ADP	A	701	-	-	X	-
2	ADP	A	702	-	-	X	-
2	ADP	B	702	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9504 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 lpg1496.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2295	1461	390	432	12	0	0	0
1	B	290	2313	1473	392	436	12	0	1	0
1	C	290	2325	1480	392	441	12	0	3	0
1	D	289	2309	1471	391	435	12	0	1	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	MET	-	initiating methionine	UNP G8UY02
A	599	LEU	-	expression tag	UNP G8UY02
A	600	GLU	-	expression tag	UNP G8UY02
A	601	HIS	-	expression tag	UNP G8UY02
A	602	HIS	-	expression tag	UNP G8UY02
A	603	HIS	-	expression tag	UNP G8UY02
A	604	HIS	-	expression tag	UNP G8UY02
A	605	HIS	-	expression tag	UNP G8UY02
A	606	HIS	-	expression tag	UNP G8UY02
B	153	MET	-	initiating methionine	UNP G8UY02
B	599	LEU	-	expression tag	UNP G8UY02
B	600	GLU	-	expression tag	UNP G8UY02
B	601	HIS	-	expression tag	UNP G8UY02
B	602	HIS	-	expression tag	UNP G8UY02
B	603	HIS	-	expression tag	UNP G8UY02
B	604	HIS	-	expression tag	UNP G8UY02
B	605	HIS	-	expression tag	UNP G8UY02
B	606	HIS	-	expression tag	UNP G8UY02
C	153	MET	-	initiating methionine	UNP G8UY02
C	599	LEU	-	expression tag	UNP G8UY02
C	600	GLU	-	expression tag	UNP G8UY02

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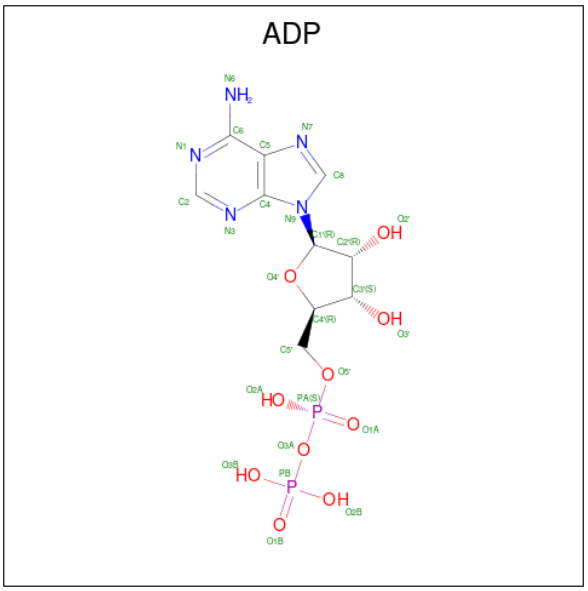
Chain	Residue	Modelled	Actual	Comment	Reference
C	601	HIS	-	expression tag	UNP G8UY02
C	602	HIS	-	expression tag	UNP G8UY02
C	603	HIS	-	expression tag	UNP G8UY02
C	604	HIS	-	expression tag	UNP G8UY02
C	605	HIS	-	expression tag	UNP G8UY02
C	606	HIS	-	expression tag	UNP G8UY02
D	153	MET	-	initiating methionine	UNP G8UY02
D	599	LEU	-	expression tag	UNP G8UY02
D	600	GLU	-	expression tag	UNP G8UY02
D	601	HIS	-	expression tag	UNP G8UY02
D	602	HIS	-	expression tag	UNP G8UY02
D	603	HIS	-	expression tag	UNP G8UY02
D	604	HIS	-	expression tag	UNP G8UY02
D	605	HIS	-	expression tag	UNP G8UY02
D	606	HIS	-	expression tag	UNP G8UY02

- 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
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
2	B	1	27	10	5	10	2	0	0

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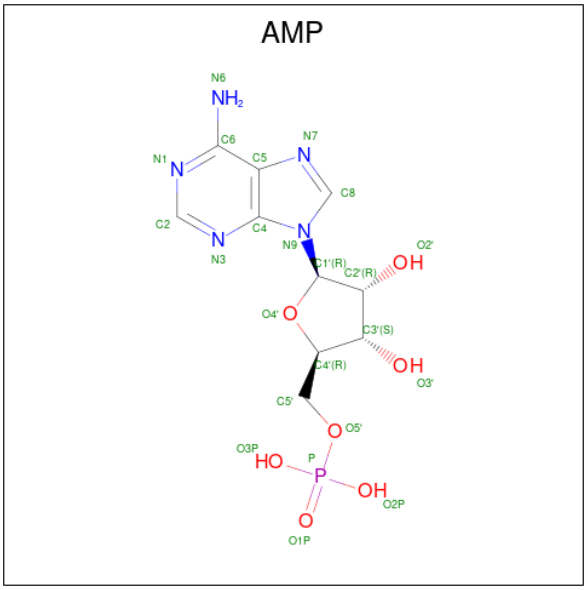
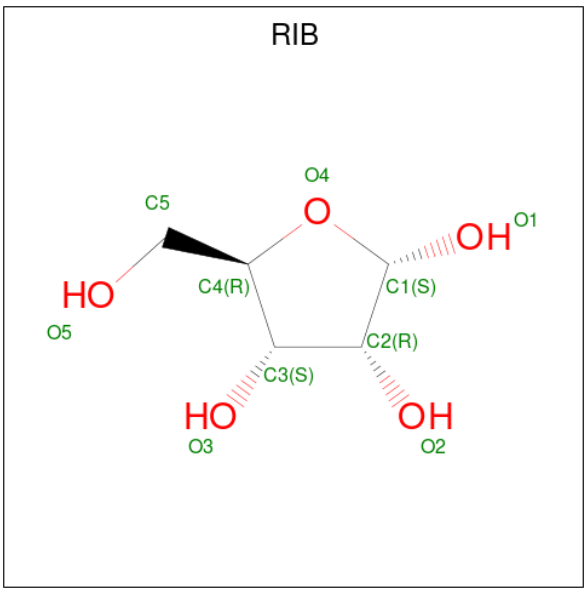
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	27	10	5	10	2	0	0

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	B	1	23	10	5	7	1	0	0

- Molecule 4 is alpha-D-ribofuranose (three-letter code: RIB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	D	1	10	5	5	0	0

- Molecule 5 is water.

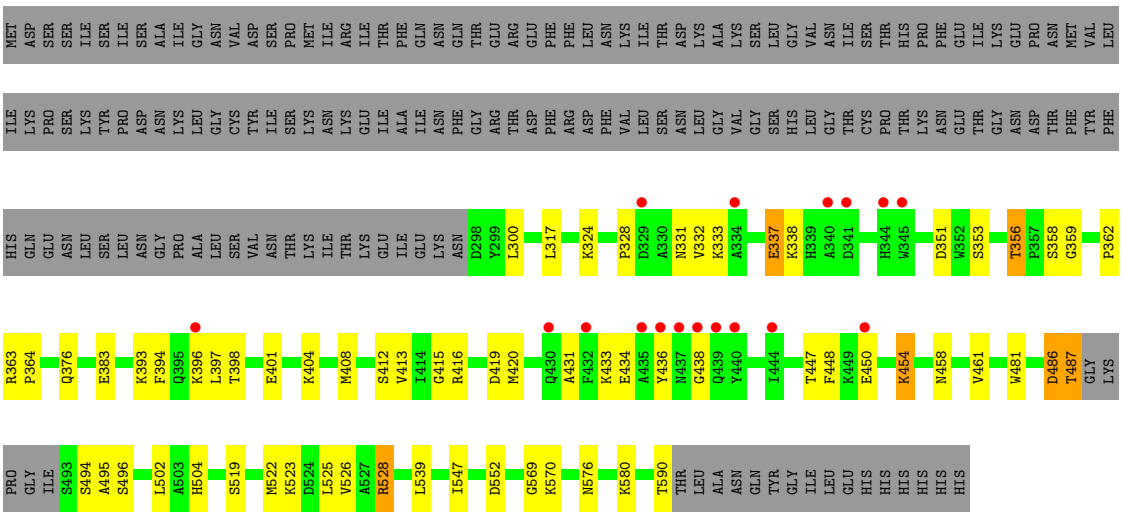
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	34	34	34	0	0
			Total	O		
5	B	28	28	28	0	0
			Total	O		
5	C	29	29	29	0	0
			Total	O		
5	D	30	30	30	0	0

3 Residue-property plots (i)

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.

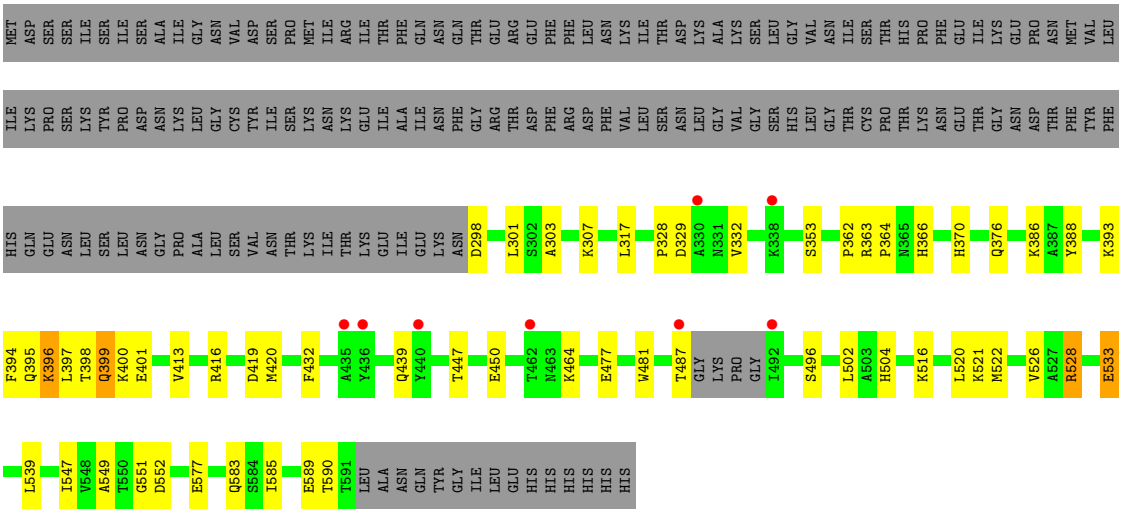
- Molecule 1: lpg1496

Chain A:



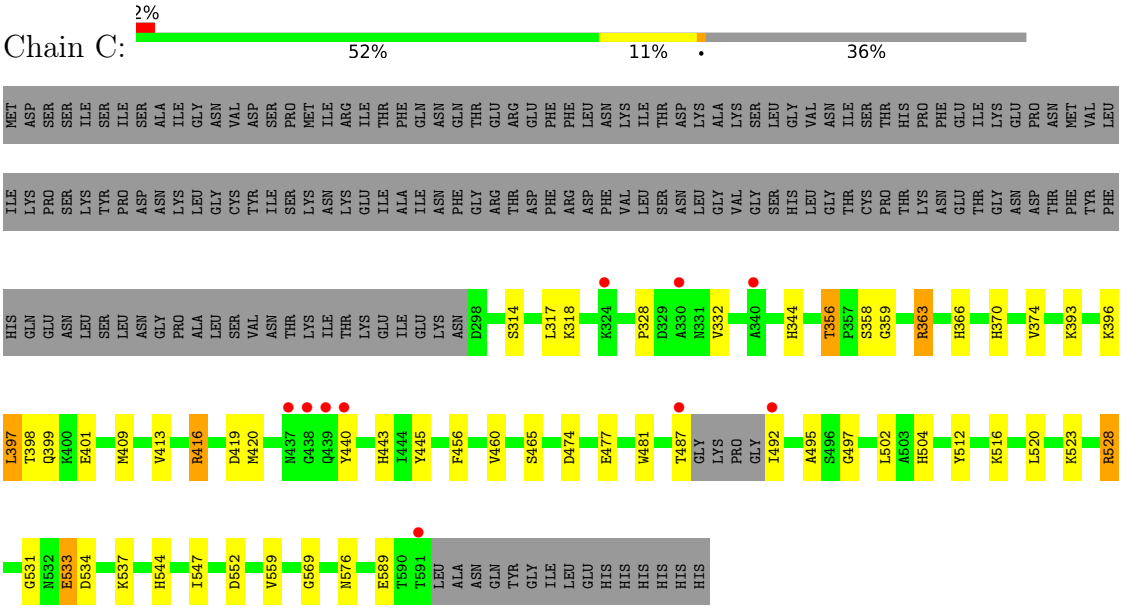
- Molecule 1: lpg1496

Chain B:



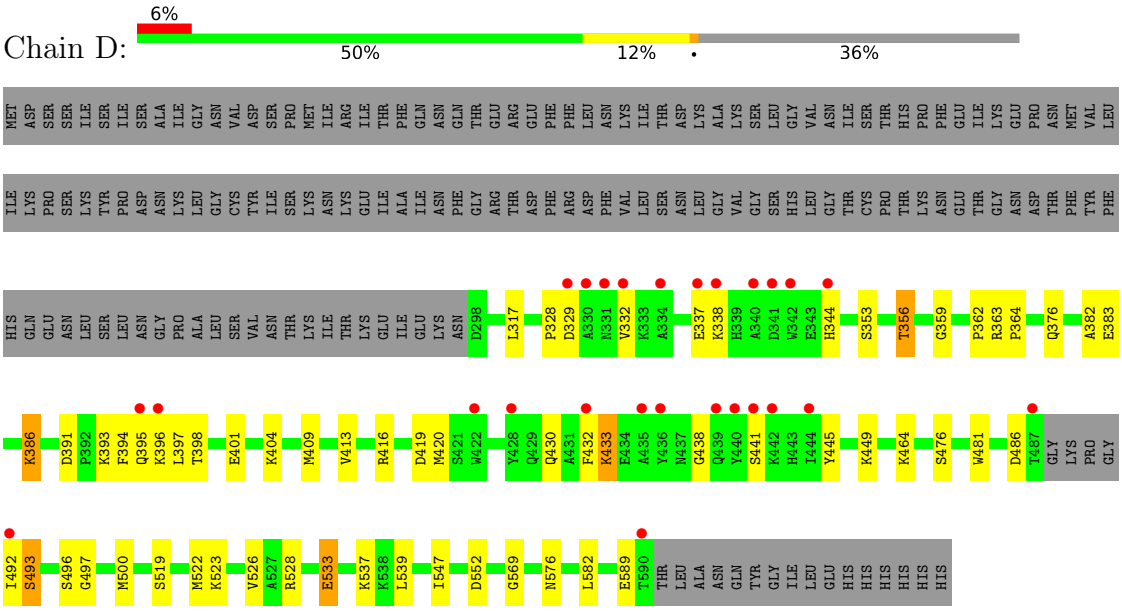
- Molecule 1: lpg1496

Chain C:



- Molecule 1: lpg1496

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	56.87Å 69.71Å 77.03Å 89.87° 72.30° 70.31°	Depositor
Resolution (Å)	34.00 – 2.11 33.29 – 2.11	Depositor EDS
% Data completeness (in resolution range)	94.3 (34.00-2.11) 94.4 (33.29-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.229 , 0.273 0.232 , 0.277	Depositor DCC
R_{free} test set	2884 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	33.5	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9504	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: RIB, ADP, AMP

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	0.40	0/2354	0.56	0/3185
1	B	0.39	0/2375	0.58	0/3214
1	C	0.38	0/2393	0.58	2/3239 (0.1%)
1	D	0.39	0/2371	0.55	0/3208
All	All	0.39	0/9493	0.57	2/12846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	416	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	C	363	ARG	NE-CZ-NH2	-5.17	117.71	120.30

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	2295	0	2222	65	1
1	B	2313	0	2245	48	0
1	C	2325	0	2252	37	0
1	D	2309	0	2239	27	1
2	A	54	0	24	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	13	0
2	C	27	0	12	4	0
3	B	23	0	12	1	0
4	D	10	0	0	0	0
5	A	34	0	0	2	0
5	B	28	0	0	2	1
5	C	29	0	0	1	0
5	D	30	0	0	0	1
All	All	9504	0	9018	175	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:549:ALA:HB2	1:B:585:ILE:HD11	1.36	1.05
1:A:393:LYS:HD2	2:A:701:ADP:N6	1.74	1.03
1:A:504:HIS:NE2	2:A:702:ADP:H2'	1.74	1.02
1:A:393:LYS:HD2	2:A:701:ADP:C6	1.95	1.01
1:B:413:VAL:HG12	2:B:702:ADP:H4'	1.39	1.01
1:B:549:ALA:CB	1:B:585:ILE:HD11	1.93	0.99
1:A:415:GLY:N	2:A:702:ADP:O1B	1.99	0.95
1:A:504:HIS:CD2	2:A:702:ADP:H2'	2.04	0.93
1:A:495:ALA:HB2	2:A:701:ADP:C2	2.07	0.89
1:A:393:LYS:CE	2:A:701:ADP:HN62	1.86	0.88
1:D:433:LYS:HD2	1:D:438:GLY:HA2	1.55	0.87
1:A:486:ASP:O	1:A:487:THR:HB	1.72	0.86
1:B:413:VAL:CG1	2:B:702:ADP:H4'	2.05	0.85
1:A:356:THR:HG21	1:A:569:GLY:HA3	1.59	0.85
1:A:393:LYS:CD	2:A:701:ADP:N6	2.40	0.84
1:A:393:LYS:NZ	2:A:701:ADP:N6	2.27	0.83
1:B:386:LYS:HE3	1:B:397:LEU:HB2	1.60	0.82
1:A:393:LYS:CE	2:A:701:ADP:N6	2.44	0.81
1:C:398:THR:OG1	1:C:401:GLU:HG2	1.82	0.79
2:C:701:ADP:O1B	2:C:701:ADP:O1A	1.99	0.79
1:B:370:HIS:HE2	2:B:702:ADP:HO3'	1.32	0.77
1:A:356:THR:CG2	1:A:569:GLY:HA3	2.16	0.76
1:B:317:LEU:O	1:B:363:ARG:HD3	1.88	0.74
1:A:393:LYS:NZ	2:A:701:ADP:HN62	1.85	0.72
1:B:547:ILE:HG23	1:B:552:ASP:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:O	2:A:702:ADP:O3B	2.07	0.72
1:A:398:THR:OG1	1:A:401:GLU:HG2	1.91	0.71
1:A:504:HIS:CD2	2:A:702:ADP:C2'	2.74	0.70
1:A:356:THR:HG21	1:A:569:GLY:CA	2.22	0.69
1:A:495:ALA:CB	2:A:701:ADP:C2	2.77	0.68
1:B:398:THR:HG22	1:B:400:LYS:H	1.59	0.68
1:B:504:HIS:ND1	2:B:702:ADP:H3'	2.07	0.67
1:A:393:LYS:HZ1	2:A:701:ADP:N6	1.93	0.67
1:C:533:GLU:OE2	1:C:537:LYS:HE3	1.95	0.67
1:D:376:GLN:HG3	1:D:582:LEU:HD13	1.75	0.66
1:A:415:GLY:CA	2:A:702:ADP:O1B	2.44	0.66
1:B:502:LEU:HD11	1:B:528:ARG:HG2	1.76	0.65
1:D:547:ILE:HG23	1:D:552:ASP:HB3	1.76	0.65
1:A:401:GLU:HG3	5:A:817:HOH:O	1.95	0.65
1:B:416:ARG:CG	2:B:702:ADP:O1A	2.45	0.65
1:C:544:HIS:HE1	1:C:559:VAL:O	1.80	0.65
1:B:413:VAL:CG1	2:B:702:ADP:O3'	2.45	0.64
1:A:433:LYS:HG2	1:A:438:GLY:HA2	1.79	0.64
1:D:356:THR:HG21	1:D:569:GLY:HA3	1.79	0.64
1:C:512:TYR:OH	2:C:701:ADP:N6	2.30	0.64
1:A:416:ARG:NH2	1:A:420:MET:O	2.31	0.64
1:A:502:LEU:HD11	1:A:528:ARG:HG2	1.78	0.64
1:C:366:HIS:HB3	1:C:413:VAL:HG11	1.79	0.64
1:B:398:THR:HB	1:B:401:GLU:HG2	1.80	0.63
1:A:547:ILE:HG23	1:A:552:ASP:HB3	1.82	0.62
1:A:495:ALA:HB2	2:A:701:ADP:N1	2.13	0.62
1:B:362:PRO:O	1:B:363:ARG:HG2	2.00	0.62
1:A:328:PRO:HB2	1:A:332:VAL:HB	1.82	0.61
1:C:397:LEU:HD13	1:C:495:ALA:HB1	1.81	0.61
1:C:547:ILE:HG23	1:C:552:ASP:HB3	1.81	0.60
1:D:533:GLU:O	1:D:537:LYS:HG2	2.01	0.60
1:B:393:LYS:HE3	3:B:701:AMP:O1P	2.02	0.60
1:B:388:TYR:OH	1:B:590:THR:O	2.20	0.59
1:B:504:HIS:CE1	2:B:702:ADP:H3'	2.37	0.59
1:A:393:LYS:HE3	2:A:701:ADP:HN62	1.67	0.59
1:D:356:THR:CG2	1:D:569:GLY:HA3	2.33	0.59
1:D:393:LYS:NZ	1:D:493:SER:O	2.34	0.59
1:C:504:HIS:CD2	2:C:701:ADP:H3'	2.38	0.58
1:D:409:MET:HE3	1:D:500:MET:HB3	1.85	0.58
1:B:522:MET:O	1:B:526:VAL:HG23	2.03	0.58
1:C:492:ILE:HA	1:C:497:GLY:HA3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:TRP:HH2	1:A:496:SER:HB3	1.68	0.57
1:D:382:ALA:O	1:D:386:LYS:HD3	2.03	0.57
1:A:333:LYS:O	1:A:337:GLU:HG2	2.04	0.57
1:C:366:HIS:NE2	2:C:701:ADP:H1'	2.19	0.57
1:C:314:SER:HA	1:C:318:LYS:HD3	1.87	0.57
1:A:447:THR:HA	1:A:450:GLU:HG2	1.87	0.57
1:C:344:HIS:HB2	5:C:825:HOH:O	2.06	0.56
2:A:702:ADP:H5'2	5:A:822:HOH:O	2.05	0.56
1:C:356:THR:HG23	1:C:358:SER:H	1.70	0.56
1:A:393:LYS:HZ1	2:A:701:ADP:HN62	1.48	0.56
1:D:356:THR:HG21	1:D:569:GLY:CA	2.36	0.56
1:A:495:ALA:HB2	2:A:701:ADP:H2	1.71	0.55
1:A:353:SER:O	1:B:464:LYS:NZ	2.40	0.55
1:C:328:PRO:HB2	1:C:332:VAL:HB	1.90	0.53
1:B:447:THR:HA	1:B:450:GLU:HG2	1.90	0.53
1:B:416:ARG:HG2	2:B:702:ADP:O1A	2.09	0.53
1:A:362:PRO:O	1:A:363:ARG:HG2	2.09	0.52
1:C:374:VAL:HB	1:C:409:MET:CE	2.40	0.52
1:A:416:ARG:NH1	2:A:702:ADP:O4'	2.43	0.52
1:B:366:HIS:NE2	2:B:702:ADP:H1'	2.25	0.51
1:B:413:VAL:HG13	2:B:702:ADP:O3'	2.10	0.51
1:A:486:ASP:O	1:A:487:THR:CB	2.53	0.51
1:B:303:ALA:O	1:B:307:LYS:HD3	2.11	0.51
1:B:516:LYS:O	1:B:520:LEU:HB2	2.11	0.51
1:D:492:ILE:HA	1:D:497:GLY:HA3	1.93	0.51
1:D:481:TRP:HH2	1:D:496:SER:HB3	1.76	0.51
1:A:519:SER:O	1:A:523:LYS:HG3	2.12	0.50
1:C:356:THR:HG22	1:C:359:GLY:O	2.11	0.50
1:B:394:PHE:C	1:B:396:LYS:H	2.13	0.50
1:B:393:LYS:O	1:B:396:LYS:HG2	2.12	0.50
1:C:502:LEU:HD11	1:C:528:ARG:HG2	1.92	0.49
1:B:533:GLU:H	1:B:533:GLU:CD	2.14	0.49
1:C:366:HIS:HB3	1:C:413:VAL:CG1	2.42	0.49
1:D:391:ASP:O	1:D:395:GLN:NE2	2.45	0.49
1:B:398:THR:HG22	1:B:399:GLN:N	2.28	0.49
1:D:522:MET:O	1:D:526:VAL:HG23	2.12	0.49
1:D:416:ARG:NH2	1:D:420:MET:O	2.42	0.49
1:A:522:MET:O	1:A:526:VAL:HG23	2.12	0.49
1:A:324:LYS:HG3	1:C:531:GLY:HA3	1.94	0.49
1:C:370:HIS:CD2	1:C:413:VAL:HG21	2.47	0.49
1:C:477:GLU:O	1:C:481:TRP:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:LYS:O	1:C:520:LEU:HB2	2.13	0.49
1:A:356:THR:HG22	1:A:358:SER:H	1.78	0.49
1:C:363:ARG:NH2	1:C:416:ARG:O	2.44	0.48
1:D:317:LEU:O	1:D:363:ARG:HD3	2.13	0.48
1:C:393:LYS:O	1:C:396:LYS:HB3	2.14	0.48
1:C:317:LEU:O	1:C:363:ARG:HD3	2.13	0.48
1:C:413:VAL:O	1:C:413:VAL:HG12	2.13	0.48
1:B:416:ARG:HD2	2:B:702:ADP:O1A	2.14	0.47
1:B:549:ALA:HB3	1:B:585:ILE:HD11	1.92	0.47
1:A:393:LYS:O	1:A:396:LYS:HB3	2.14	0.47
1:C:416:ARG:NH2	1:C:420:MET:O	2.40	0.47
1:B:549:ALA:CB	1:B:585:ILE:CD1	2.81	0.47
1:C:356:THR:HG21	1:C:569:GLY:HA3	1.97	0.46
1:C:443:HIS:CE1	1:C:445:TYR:HB2	2.51	0.46
1:A:431:ALA:HA	1:A:434:GLU:HB2	1.97	0.46
1:B:393:LYS:NZ	1:C:474[B]:ASP:OD1	2.46	0.46
1:B:551:GLY:HA2	5:B:806:HOH:O	2.16	0.46
1:A:413:VAL:HG12	2:A:702:ADP:H4'	1.97	0.45
1:C:456:PHE:O	1:C:460:VAL:HG13	2.15	0.45
1:C:356:THR:HG21	1:C:569:GLY:CA	2.46	0.45
1:D:394:PHE:C	1:D:396:LYS:H	2.20	0.45
1:B:481:TRP:HH2	1:B:496:SER:HB3	1.82	0.45
1:A:458:ASN:O	1:A:461:VAL:HG12	2.16	0.45
1:B:353:SER:HA	1:B:364:PRO:HD3	1.98	0.45
1:B:393:LYS:NZ	1:C:474[A]:ASP:OD1	2.47	0.45
1:A:525:LEU:HD11	1:A:539:LEU:HD23	1.99	0.45
1:B:432:PHE:HE1	1:B:439:GLN:HG3	1.82	0.45
1:A:351:ASP:O	1:A:364:PRO:HD2	2.17	0.45
1:A:317:LEU:O	1:A:363:ARG:HD3	2.16	0.44
1:D:353:SER:HA	1:D:364:PRO:HD3	1.98	0.44
1:B:521:LYS:HA	1:B:521:LYS:HD3	1.82	0.44
1:A:404:LYS:O	1:A:408:MET:HG2	2.18	0.44
1:B:362:PRO:C	1:B:363:ARG:HG2	2.38	0.44
1:D:328:PRO:HB2	1:D:332:VAL:HB	2.00	0.44
1:A:356:THR:HB	1:A:359:GLY:O	2.17	0.44
1:B:328:PRO:HB2	1:B:332:VAL:HB	2.00	0.44
1:A:494:SER:HA	2:A:701:ADP:C5	2.53	0.43
1:A:362:PRO:C	1:A:363:ARG:HG2	2.38	0.43
1:C:533:GLU:OE2	1:C:537:LYS:CE	2.65	0.43
1:D:519:SER:O	1:D:523:LYS:HG3	2.18	0.43
1:D:356:THR:HB	1:D:359:GLY:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:PHE:O	1:A:397:LEU:HB2	2.19	0.43
1:B:370:HIS:HE1	5:B:809:HOH:O	2.01	0.43
1:C:533:GLU:O	1:C:537:LYS:HG2	2.18	0.43
1:A:396:LYS:HG2	1:A:396:LYS:O	2.19	0.43
1:A:300:LEU:HD12	1:A:376:GLN:HE21	1.83	0.43
1:A:481:TRP:CH2	1:A:496:SER:HB3	2.51	0.43
1:D:409:MET:HE2	1:D:500:MET:HE3	2.01	0.42
1:A:570:LYS:HE2	1:A:570:LYS:HB3	1.84	0.42
1:B:416:ARG:NH2	1:B:420:MET:O	2.48	0.42
1:C:370:HIS:HD2	1:C:413:VAL:HG21	1.84	0.42
1:D:398:THR:OG1	1:D:401[A]:GLU:HG2	2.20	0.42
1:D:445:TYR:O	1:D:449:LYS:HG3	2.20	0.42
1:B:301:LEU:HD21	1:B:583:GLN:NE2	2.35	0.42
1:A:454:LYS:HB2	1:A:454:LYS:HE2	1.55	0.41
1:B:298:ASP:OD2	1:B:376:GLN:NE2	2.53	0.41
1:C:374:VAL:HB	1:C:409:MET:HE3	2.02	0.41
1:A:353:SER:HA	1:A:364:PRO:HD3	2.02	0.41
1:A:415:GLY:HA3	1:A:448:PHE:O	2.19	0.41
1:A:328:PRO:HG2	1:A:333:LYS:HG3	2.02	0.41
1:A:415:GLY:HA3	2:A:702:ADP:O1B	2.19	0.41
1:B:413:VAL:HG12	2:B:702:ADP:C4'	2.28	0.41
1:B:416:ARG:CD	2:B:702:ADP:O1A	2.69	0.41
1:A:331:ASN:HB2	1:A:436:TYR:OH	2.21	0.40
1:D:362:PRO:O	1:D:363:ARG:HG2	2.22	0.40
1:D:401[A]:GLU:OE1	1:D:404:LYS:NZ	2.44	0.40
1:D:432:PHE:CE1	1:D:441:SER:HB3	2.57	0.40
1:A:486:ASP:HB3	1:A:487:THR:H	1.80	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:826:HOH:O	5:D:829:HOH:O[1_565]	1.50	0.70
1:A:393:LYS:NZ	1:D:476:SER:OG[1_556]	2.10	0.10

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/454 (63%)	277 (98%)	7 (2%)	0	100	100
1	B	287/454 (63%)	281 (98%)	6 (2%)	0	100	100
1	C	289/454 (64%)	283 (98%)	6 (2%)	0	100	100
1	D	286/454 (63%)	278 (97%)	7 (2%)	1 (0%)	41	40
All	All	1146/1816 (63%)	1119 (98%)	26 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	397	LEU

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	245/394 (62%)	233 (95%)	12 (5%)	25	22
1	B	248/394 (63%)	236 (95%)	12 (5%)	25	23
1	C	250/394 (64%)	237 (95%)	13 (5%)	23	20
1	D	247/394 (63%)	228 (92%)	19 (8%)	13	9
All	All	990/1576 (63%)	934 (94%)	56 (6%)	20	17

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	337	GLU
1	A	338	LYS
1	A	356	THR
1	A	383	GLU
1	A	419	ASP
1	A	454	LYS
1	A	486	ASP
1	A	487	THR
1	A	528	ARG
1	A	576	ASN
1	A	580	LYS
1	A	590	THR
1	B	329	ASP
1	B	395	GLN
1	B	396	LYS
1	B	399	GLN
1	B	419	ASP
1	B	477	GLU
1	B	487	THR
1	B	528	ARG
1	B	533	GLU
1	B	539	LEU
1	B	577	GLU
1	B	589	GLU
1	C	356	THR
1	C	397	LEU
1	C	399	GLN
1	C	419	ASP
1	C	440	TYR
1	C	465	SER
1	C	487	THR
1	C	523	LYS
1	C	528	ARG
1	C	533	GLU
1	C	534	ASP
1	C	576	ASN
1	C	589	GLU
1	D	329	ASP
1	D	337	GLU
1	D	338	LYS
1	D	344	HIS
1	D	356	THR
1	D	383	GLU

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Mol	Chain	Res	Type
1	D	386	LYS
1	D	413	VAL
1	D	419	ASP
1	D	430	GLN
1	D	433	LYS
1	D	464	LYS
1	D	486	ASP
1	D	493	SER
1	D	528	ARG
1	D	533	GLU
1	D	539	LEU
1	D	576	ASN
1	D	589	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN
1	A	376	GLN
1	A	427	HIS
1	A	583	GLN
1	B	344	HIS
1	B	583	GLN
1	C	315	ASN
1	C	437	ASN
1	C	504	HIS
1	C	544	HIS
1	D	350	GLN
1	D	430	GLN

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)

6 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	702	-	24,29,29	1.16	2 (8%)	29,45,45	1.79	10 (34%)
3	AMP	B	701	-	22,25,25	1.03	1 (4%)	25,38,38	1.46	4 (16%)
4	RIB	D	701	-	10,10,10	1.00	1 (10%)	13,14,14	1.92	5 (38%)
2	ADP	A	702	-	24,29,29	1.04	1 (4%)	29,45,45	1.63	4 (13%)
2	ADP	C	701	-	24,29,29	1.17	2 (8%)	29,45,45	1.81	7 (24%)
2	ADP	A	701	-	24,29,29	1.04	2 (8%)	29,45,45	1.48	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	702	-	-	3/12/32/32	0/3/3/3
3	AMP	B	701	-	-	4/6/26/26	0/3/3/3
4	RIB	D	701	-	-	0/2/18/18	0/1/1/1
2	ADP	A	702	-	-	4/12/32/32	0/3/3/3
2	ADP	C	701	-	-	6/12/32/32	0/3/3/3
2	ADP	A	701	-	-	2/12/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	ADP	C5-C4	2.97	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	702	ADP	C5-C4	2.70	1.48	1.40
2	A	702	ADP	C5-C4	2.61	1.47	1.40
2	C	701	ADP	C2-N3	2.55	1.36	1.32
4	D	701	RIB	C1-C2	-2.47	1.49	1.52
3	B	701	AMP	C5-C4	2.46	1.47	1.40
2	A	701	ADP	O4'-C1'	2.45	1.44	1.41
2	B	702	ADP	C2-N3	2.32	1.35	1.32
2	A	701	ADP	C5-C4	2.22	1.46	1.40

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	ADP	PA-O3A-PB	-5.03	115.55	132.83
2	A	702	ADP	C3'-C2'-C1'	4.26	107.40	100.98
2	A	702	ADP	PA-O3A-PB	-4.13	118.67	132.83
3	B	701	AMP	N3-C2-N1	-3.90	122.58	128.68
2	B	702	ADP	N3-C2-N1	-3.75	122.81	128.68
2	B	702	ADP	PA-O3A-PB	-3.62	120.42	132.83
4	D	701	RIB	O2-C2-C1	-3.57	101.96	111.82
2	A	701	ADP	N3-C2-N1	-3.37	123.41	128.68
2	C	701	ADP	N3-C2-N1	-3.13	123.79	128.68
2	A	701	ADP	C3'-C2'-C1'	3.08	105.62	100.98
2	A	702	ADP	N3-C2-N1	-2.97	124.04	128.68
2	A	701	ADP	PA-O3A-PB	-2.89	122.90	132.83
4	D	701	RIB	C5-C4-C3	-2.87	108.16	115.09
2	C	701	ADP	O3'-C3'-C4'	-2.86	102.78	111.05
2	B	702	ADP	O3'-C3'-C4'	-2.81	102.92	111.05
2	B	702	ADP	C4-C5-N7	-2.79	106.49	109.40
3	B	701	AMP	C3'-C2'-C1'	2.68	105.02	100.98
2	C	701	ADP	N6-C6-N1	2.58	123.93	118.57
3	B	701	AMP	O5'-P-O1P	-2.56	99.29	106.47
2	A	702	ADP	C4-C5-N7	-2.56	106.74	109.40
2	B	702	ADP	C2'-C3'-C4'	2.55	107.59	102.64
4	D	701	RIB	C1-C2-C3	2.54	105.48	102.30
2	B	702	ADP	O4'-C1'-C2'	2.48	110.55	106.93
2	B	702	ADP	C1'-N9-C4	-2.45	122.33	126.64
2	B	702	ADP	C2-N1-C6	2.43	122.91	118.75
2	C	701	ADP	C1'-N9-C4	2.29	130.66	126.64
2	A	701	ADP	C2'-C3'-C4'	2.27	107.06	102.64
2	B	702	ADP	O3B-PB-O2B	2.26	116.27	107.64
4	D	701	RIB	C2-C3-C4	2.16	106.83	102.64
4	D	701	RIB	O1-C1-O4	-2.13	108.40	111.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	ADP	O2'-C2'-C1'	-2.11	103.05	110.85
3	B	701	AMP	C4-C5-N7	-2.11	107.20	109.40
2	C	701	ADP	C3'-C2'-C1'	-2.06	97.88	100.98
2	B	702	ADP	O2A-PA-O1A	2.04	122.32	112.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	702	ADP	C5'-O5'-PA-O2A
2	C	701	ADP	C3'-C4'-C5'-O5'
3	B	701	AMP	C5'-O5'-P-O1P
3	B	701	AMP	C5'-O5'-P-O2P
3	B	701	AMP	C5'-O5'-P-O3P
2	B	702	ADP	O4'-C4'-C5'-O5'
2	B	702	ADP	C3'-C4'-C5'-O5'
2	C	701	ADP	O4'-C4'-C5'-O5'
2	B	702	ADP	C4'-C5'-O5'-PA
2	A	701	ADP	C4'-C5'-O5'-PA
2	C	701	ADP	PA-O3A-PB-O2B
2	A	702	ADP	C5'-O5'-PA-O3A
2	A	702	ADP	C5'-O5'-PA-O1A
2	C	701	ADP	C5'-O5'-PA-O2A
2	C	701	ADP	PB-O3A-PA-O1A
2	C	701	ADP	C5'-O5'-PA-O3A
2	A	701	ADP	O4'-C4'-C5'-O5'
3	B	701	AMP	O4'-C4'-C5'-O5'
2	A	702	ADP	PB-O3A-PA-O1A

There are no ring outliers.

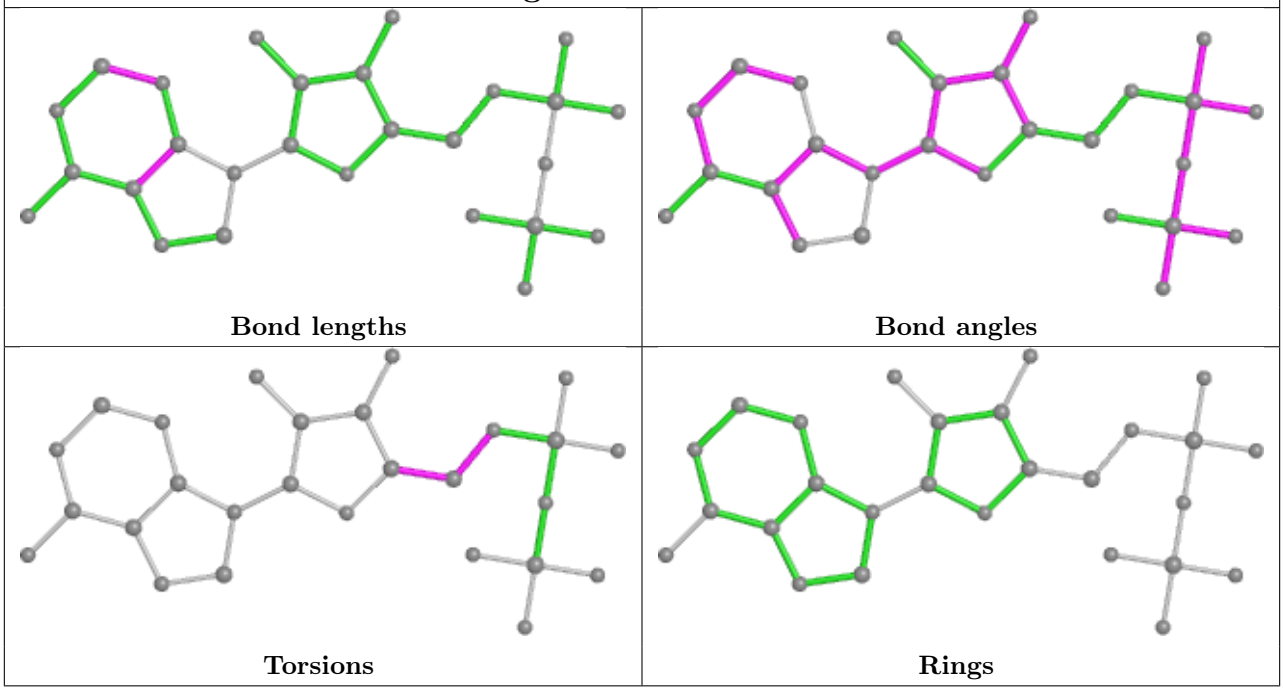
5 monomers are involved in 43 short contacts:

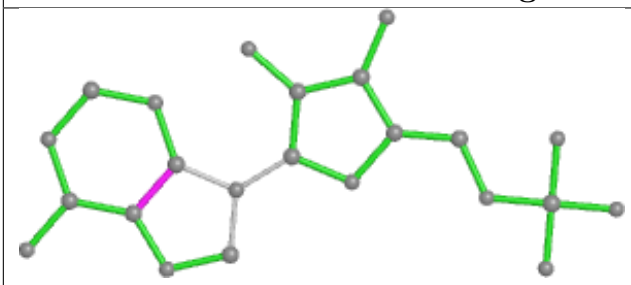
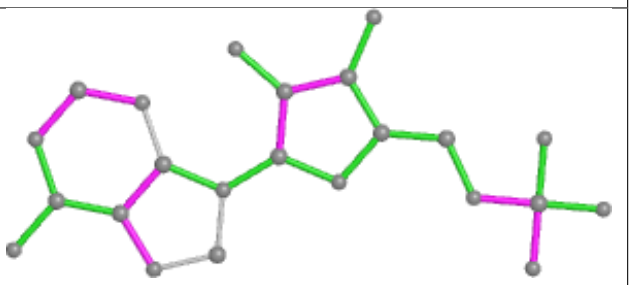
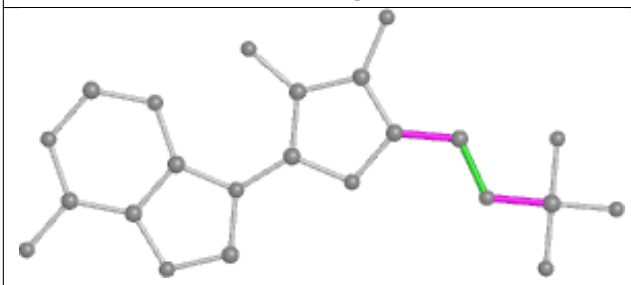
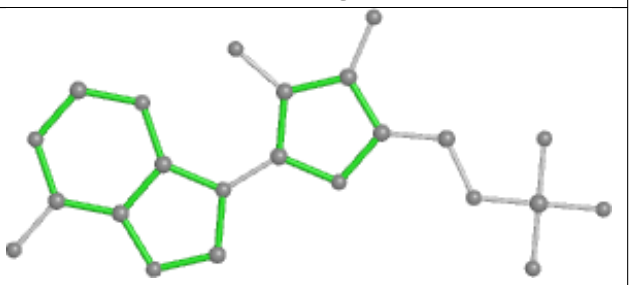
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	702	ADP	13	0
3	B	701	AMP	1	0
2	A	702	ADP	10	0
2	C	701	ADP	4	0
2	A	701	ADP	15	0

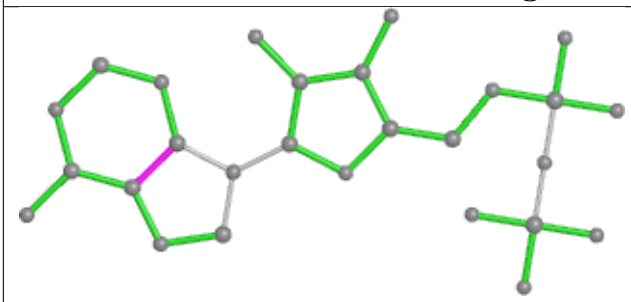
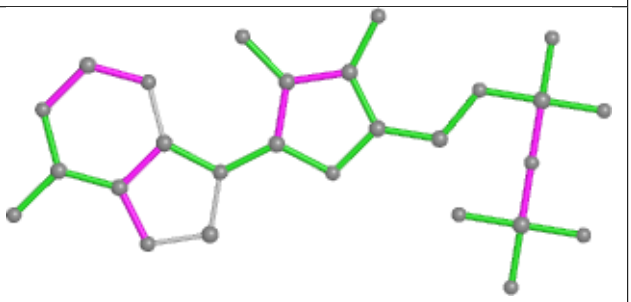
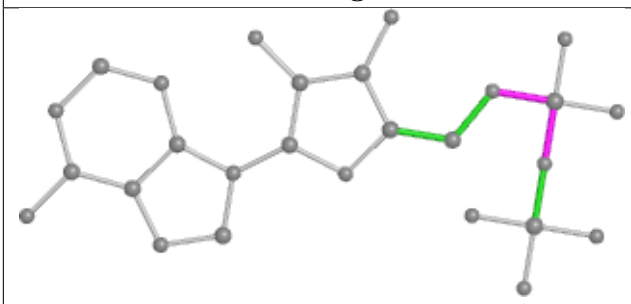
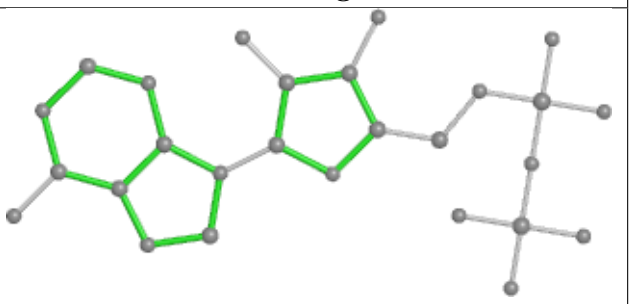
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

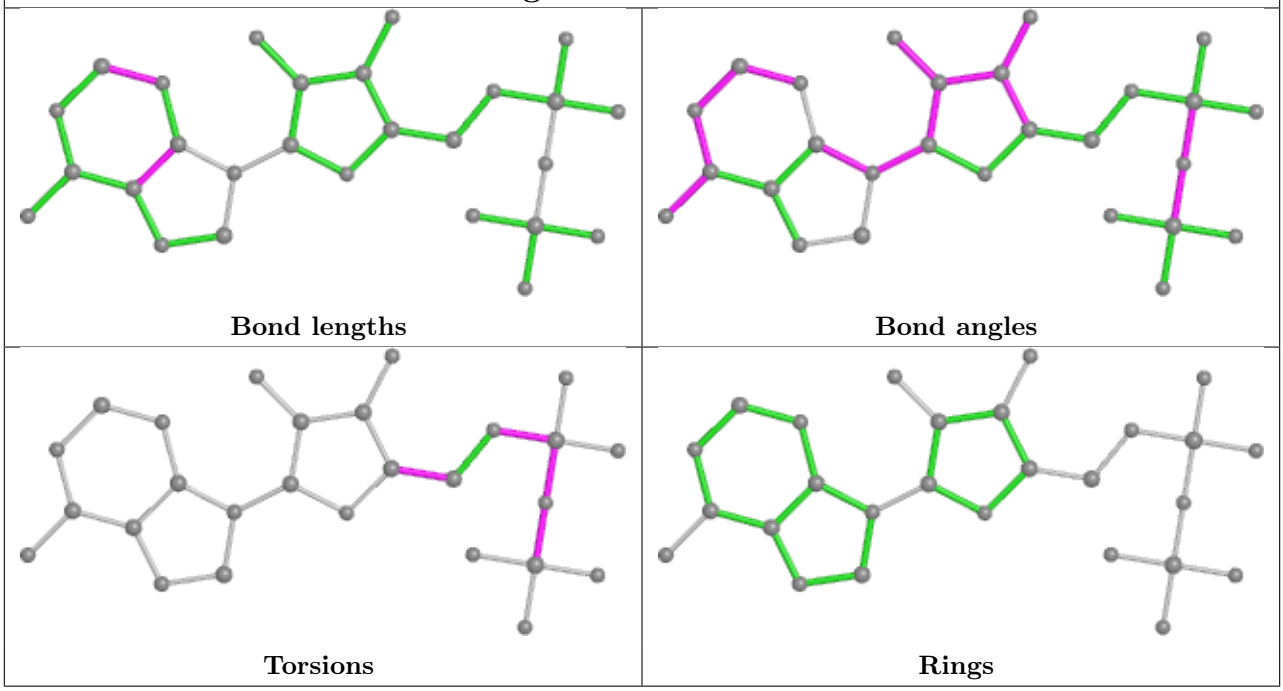
Ligand ADP B 702



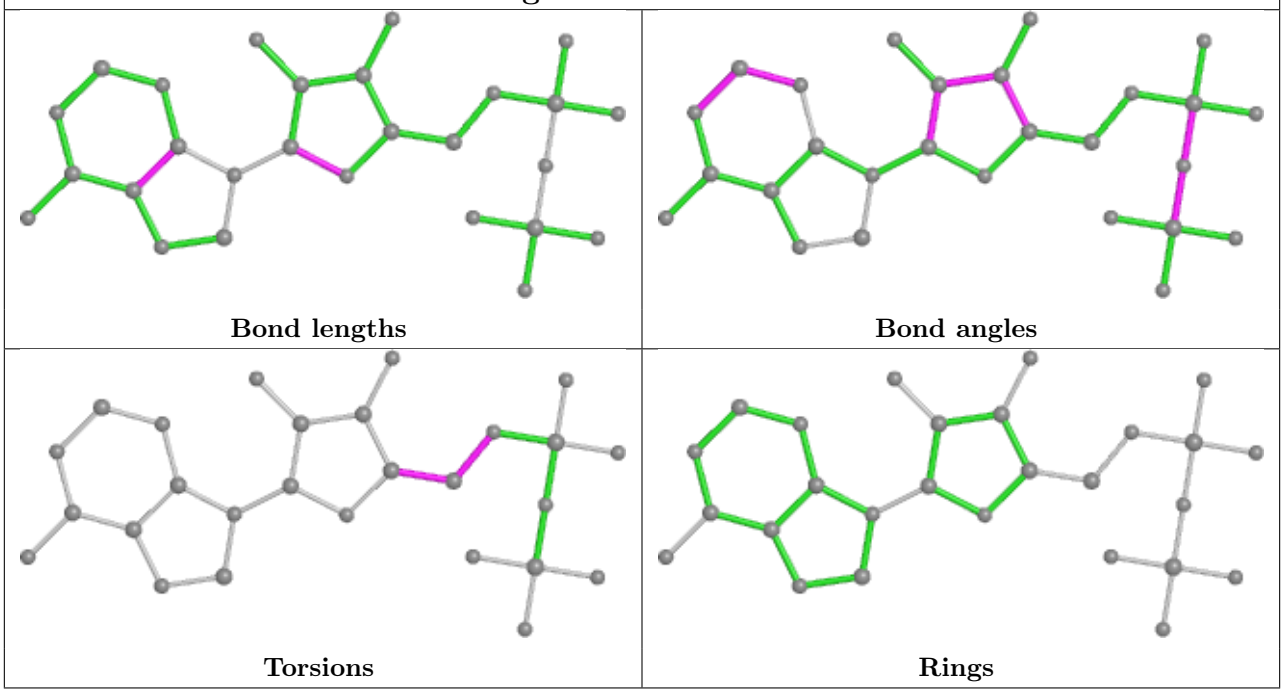
Ligand AMP B 701	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 702	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP C 701



Ligand ADP A 701



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	288/454 (63%)	0.39	17 (5%)	22	27	22, 34, 64, 81	0
1	B	290/454 (63%)	0.34	8 (2%)	53	59	23, 35, 53, 66	0
1	C	290/454 (63%)	0.39	10 (3%)	45	51	23, 36, 55, 77	0
1	D	289/454 (63%)	0.43	26 (8%)	9	12	23, 35, 64, 79	0
All	All	1157/1816 (63%)	0.39	61 (5%)	26	31	22, 35, 59, 81	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	440	TYR	9.9
1	A	437	ASN	7.2
1	D	440	TYR	6.2
1	A	440	TYR	6.1
1	B	440	TYR	5.9
1	C	487	THR	5.2
1	A	436	TYR	4.9
1	A	341	ASP	4.8
1	C	437	ASN	4.5
1	C	591	THR	4.4
1	A	435	ALA	4.4
1	D	331	ASN	4.4
1	D	487	THR	4.4
1	C	340	ALA	4.3
1	A	340	ALA	4.2
1	B	492	ILE	4.1
1	D	337	GLU	3.8
1	D	330	ALA	3.8
1	D	439	GLN	3.6
1	C	438	GLY	3.5
1	D	344	HIS	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	590	THR	3.4
1	D	341	ASP	3.2
1	D	444	ILE	3.1
1	A	396	LYS	3.1
1	D	334	ALA	3.1
1	A	344	HIS	3.0
1	A	444	ILE	3.0
1	B	487	THR	2.9
1	B	330	ALA	2.9
1	D	340	ALA	2.9
1	C	492	ILE	2.8
1	B	436	TYR	2.8
1	D	332	VAL	2.7
1	D	342	TRP	2.7
1	D	428	TYR	2.7
1	C	439	GLN	2.6
1	A	438	GLY	2.6
1	D	395	GLN	2.6
1	A	450	GLU	2.6
1	D	441	SER	2.6
1	B	435	ALA	2.5
1	A	334	ALA	2.5
1	B	462	THR	2.4
1	A	439	GLN	2.4
1	A	345	TRP	2.4
1	A	430	GLN	2.3
1	A	432	PHE	2.3
1	D	492	ILE	2.3
1	D	329	ASP	2.2
1	D	396	LYS	2.2
1	B	338	LYS	2.2
1	D	442	LYS	2.2
1	D	432	PHE	2.1
1	D	436	TYR	2.1
1	C	330	ALA	2.1
1	C	324	LYS	2.1
1	A	329	ASP	2.1
1	D	435	ALA	2.1
1	D	338	LYS	2.0
1	D	422	TRP	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)

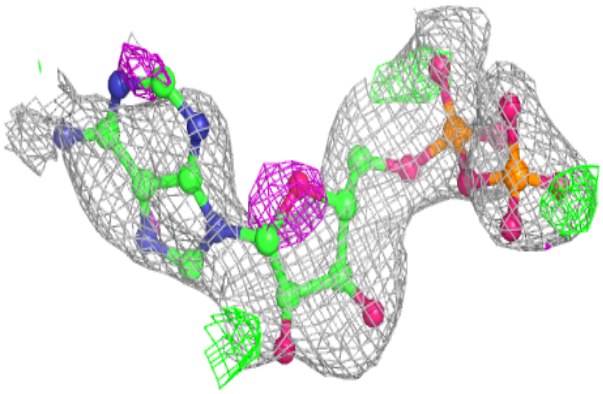
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

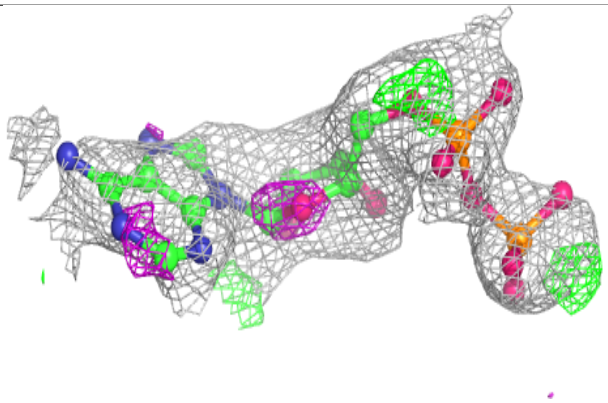
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ADP	A	701	27/27	0.62	0.27	36,62,67,69	8
2	ADP	B	702	27/27	0.72	0.27	32,35,43,46	8
2	ADP	A	702	27/27	0.73	0.27	35,41,45,47	8
2	ADP	C	701	27/27	0.76	0.27	33,35,40,40	8
4	RIB	D	701	10/10	0.84	0.17	33,34,37,37	0
3	AMP	B	701	23/23	0.85	0.14	40,55,60,62	4

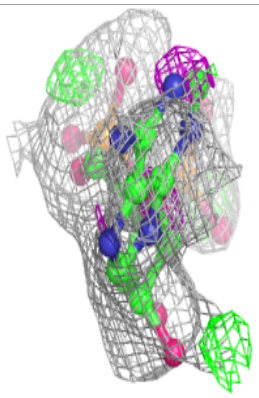
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 701:

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

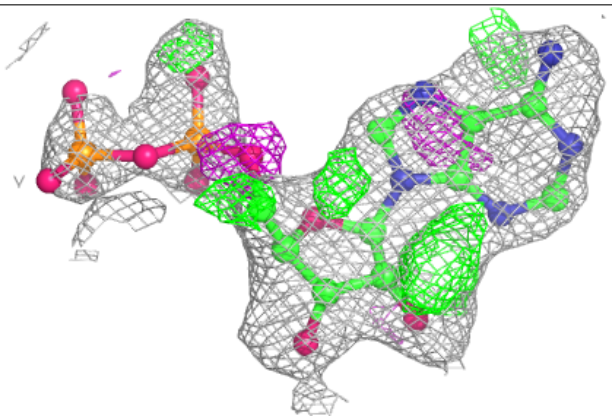


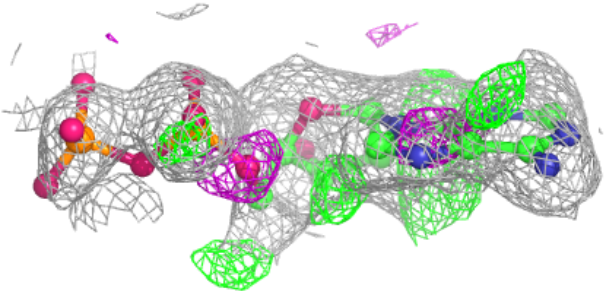


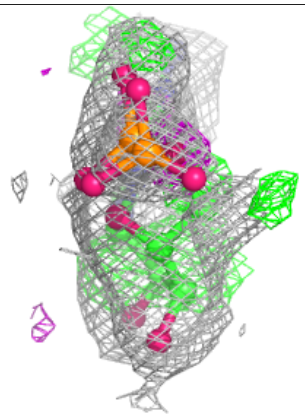


Electron density around ADP B 702:

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

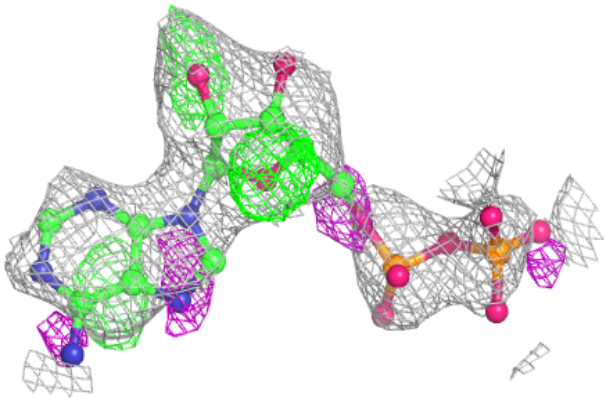


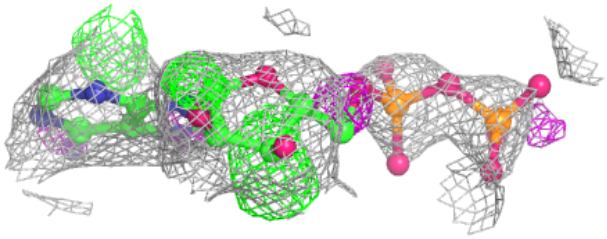


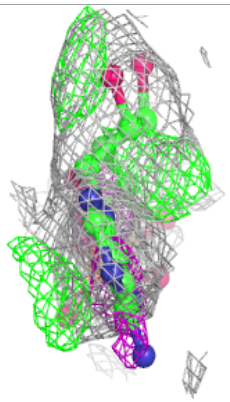


Electron density around ADP A 702:

$2mF_o$-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 701:

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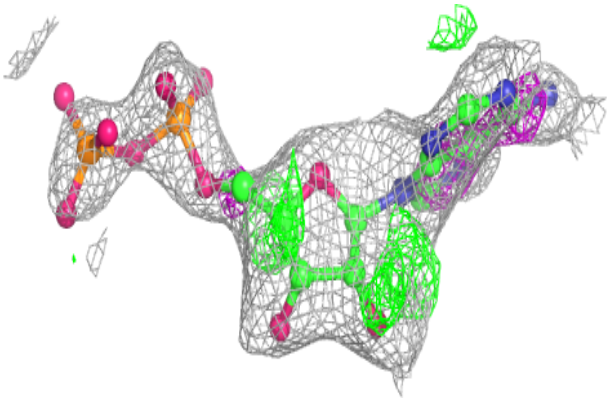
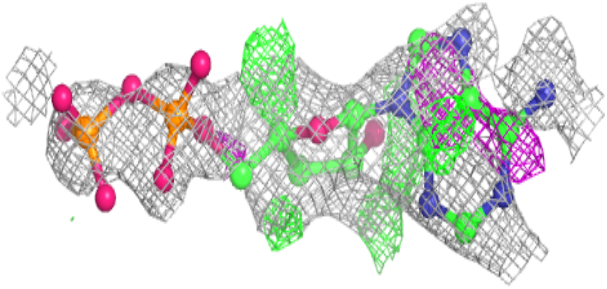
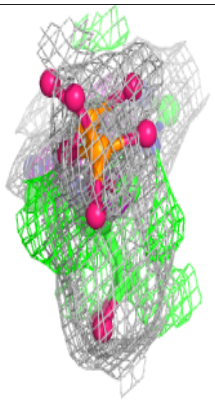
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around AMP B 701:

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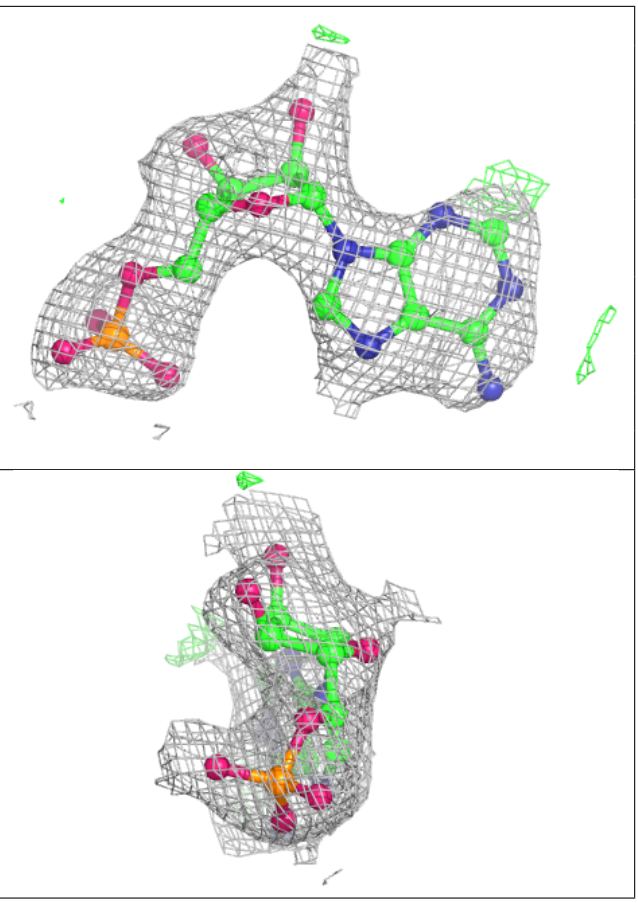
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.