Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 07:40 AM EDT

PDB ID	:	2IS6
Title	:	Crystal structure of UvrD-DNA-ADPMgF3 ternary complex
Authors	:	Yang, W.; Lee, J.Y.
Deposited on	:	2006-10-16
Resolution	:	2.20 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:

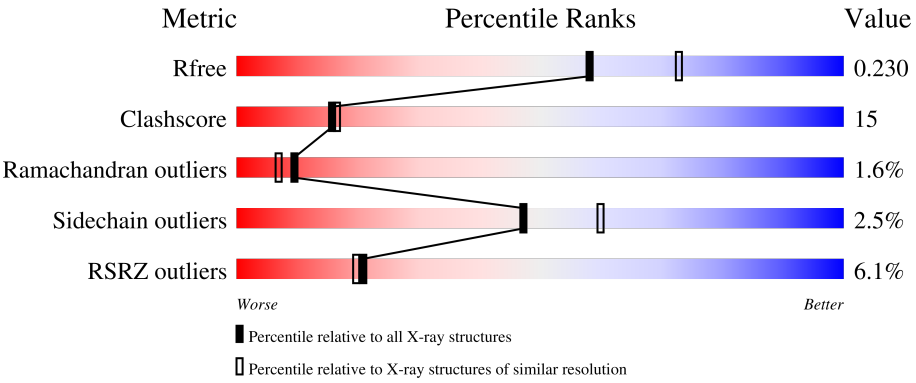
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	C	25	4% 32% 60% 8%
1	D	25	4% 32% 60% 8%
2	A	680	6% 71% 23%
2	B	680	6% 68% 26%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11795 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 DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*GP*TP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			
1	D	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	654	Total	C	N	O	S	0	0	0
			5155	3224	939	966	26			
2	B	652	Total	C	N	O	S	0	0	0
			5127	3208	930	962	27			

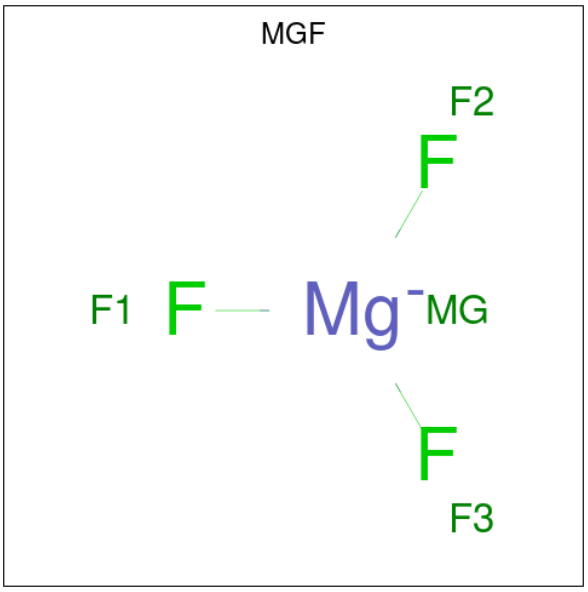
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	engineered mutation	UNP P03018
B	399	VAL	ALA	engineered mutation	UNP P03018

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

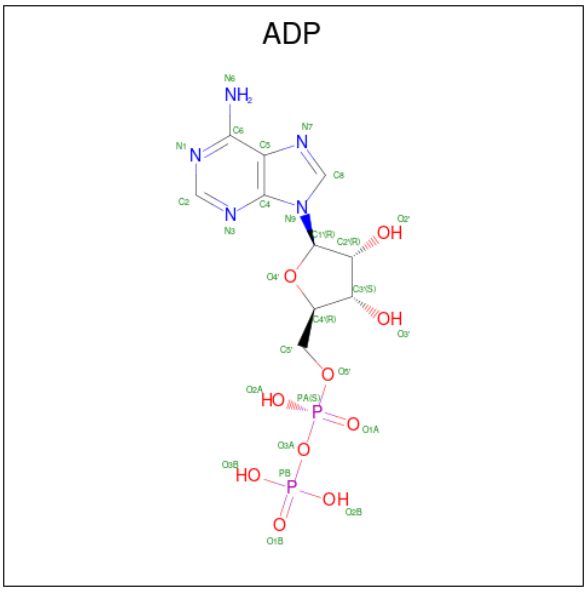
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F_3Mg).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total F Mg 4 3 1	0	0
4	B	1	Total F Mg 4 3 1	0	0

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



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

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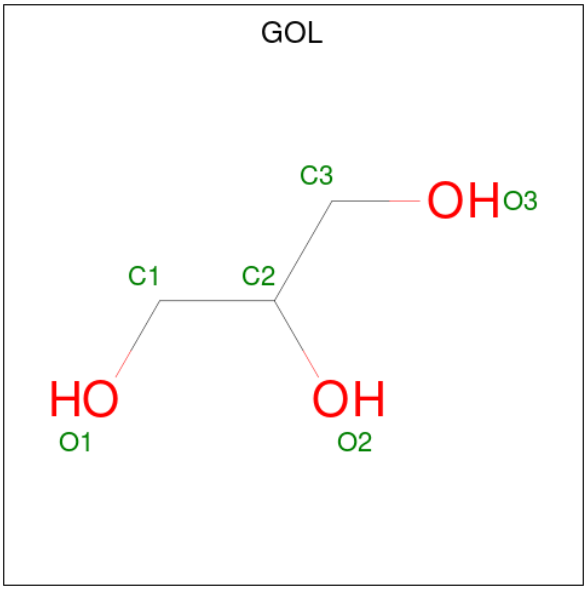
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

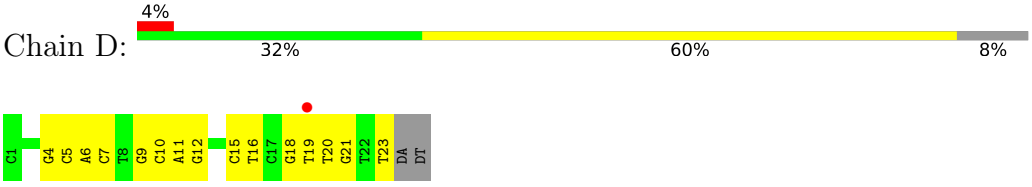
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	15	Total	O	0	0
			15	15		
7	D	10	Total	O	0	0
			10	10		
7	A	243	Total	O	0	0
			243	243		
7	B	239	Total	O	0	0
			239	239		

3 Residue-property plots (i)

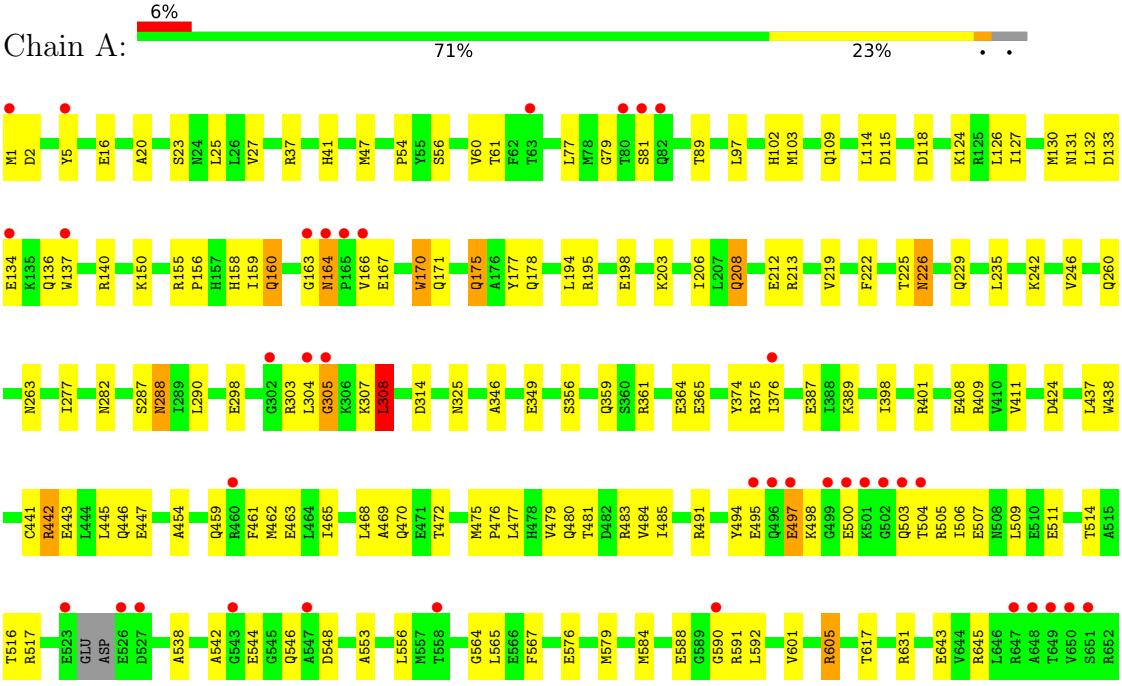
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

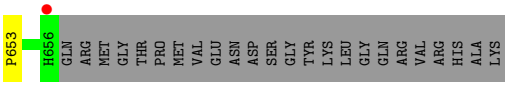
• Molecule 1: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*GP*TP*TP*AP*T)-3'

• Molecule 1: 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*GP*TP*TP*AP*T)-3'



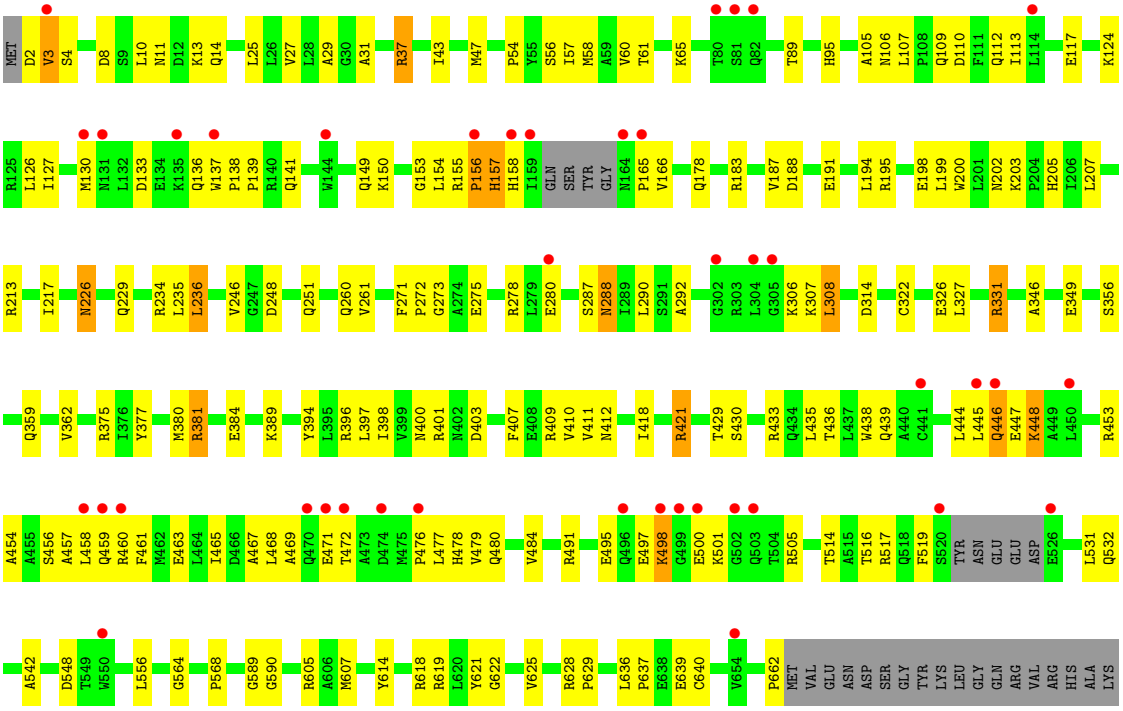
• Molecule 2: DNA helicase II





• Molecule 2: DNA helicase II

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.34Å 96.61Å 110.93Å 90.00° 94.05° 90.00°	Depositor
Resolution (Å)	29.94 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.94-2.20) 89.2 (48.01-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.63 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.240 0.202 , 0.230	Depositor DCC
R_{free} test set	9797 reflections (9.59%)	wwPDB-VP
Wilson B-factor (Å^2)	37.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11795	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GOL, ADP, MGF

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	C	0.30	0/523	0.73	0/806
1	D	0.29	0/523	0.71	0/806
2	A	0.33	0/5251	0.57	1/7107 (0.0%)
2	B	0.34	0/5220	0.54	1/7062 (0.0%)
All	All	0.33	0/11517	0.57	2/15781 (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})
2	B	662	PRO	N-CA-CB	5.71	110.15	103.30
2	A	653	PRO	N-CA-CB	5.35	109.72	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	468	0	262	14	0
1	D	468	0	262	24	0
2	A	5155	0	4971	135	0
2	B	5127	0	4969	152	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	6	0	8	2	0
7	A	243	0	0	5	0
7	B	239	0	0	11	0
7	C	15	0	0	1	0
7	D	10	0	0	0	0
All	All	11795	0	10496	320	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 15.

All (320) 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:D:4:DG:H2"	1:D:5:DC:H5"	1.38	0.99
1:D:5:DC:H2"	1:D:6:DA:C8	2.07	0.90
1:C:18:DG:H2"	1:C:19:DT:H5'	1.52	0.89
2:A:155:ARG:H	2:A:158:HIS:HD2	1.17	0.88
2:A:401:ARG:NH1	2:A:465:ILE:HG22	1.93	0.83
2:B:375:ARG:CZ	2:B:548:ASP:HB2	2.11	0.81
2:A:23:SER:HA	2:A:242:LYS:HD2	1.62	0.80
1:C:13:DT:H2"	1:C:14:DG:C8	2.20	0.77
2:B:468:LEU:O	2:B:472:THR:HG22	1.87	0.74
2:A:475:MET:HB3	2:A:479:VAL:HG13	1.69	0.74
1:D:4:DG:C2'	1:D:5:DC:H5"	2.17	0.73
2:A:491:ARG:O	2:A:495:GLU:HG3	1.87	0.73
1:D:11:DA:H2"	1:D:12:DG:C8	2.25	0.72
1:C:18:DG:C2'	1:C:19:DT:H5'	2.19	0.72
2:A:25:LEU:HD11	2:A:277:ILE:HG13	1.72	0.72
2:A:475:MET:HB3	2:A:479:VAL:CG1	2.19	0.72
2:A:401:ARG:HH11	2:A:465:ILE:HG22	1.53	0.71
2:B:396:ARG:HD2	2:B:403:ASP:OD2	1.91	0.71
2:B:438:TRP:HZ3	2:B:465:ILE:HD12	1.56	0.70
2:A:150:LYS:NZ	2:A:178:GLN:HE22	1.89	0.70
2:B:183:ARG:HD2	2:B:435:LEU:HA	1.73	0.70
2:A:443:GLU:HA	2:A:446:GLN:HG2	1.73	0.70
1:D:6:DA:H1'	1:D:7:DC:H5"	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:GLN:CD	2:B:396:ARG:HD3	2.11	0.70
2:B:112:GLN:HG2	2:B:396:ARG:HH11	1.58	0.69
2:A:155:ARG:H	2:A:158:HIS:CD2	2.05	0.68
2:B:150:LYS:NZ	2:B:178:GLN:HE22	1.92	0.67
2:B:226:ASN:HD21	2:B:229:GLN:HG3	1.58	0.67
2:B:459:GLN:O	2:B:463:GLU:HG3	1.94	0.67
2:A:503:GLN:O	2:A:506:ILE:HG22	1.95	0.67
2:A:25:LEU:HD21	2:A:277:ILE:HD12	1.77	0.66
2:A:1:MET:H3	2:A:5:TYR:HE2	1.44	0.66
2:A:564:GLY:H	2:A:605:ARG:NH2	1.92	0.66
2:A:47:MET:CE	2:A:54:PRO:HG3	2.26	0.66
2:A:477:LEU:HG	2:A:516:THR:HB	1.77	0.65
2:B:436:THR:OG1	2:B:439:GLN:HG3	1.97	0.65
2:B:155:ARG:HB3	2:B:156:PRO:HD2	1.78	0.65
2:B:136:GLN:HE21	2:B:137:TRP:HE1	1.45	0.64
2:A:260:GLN:HG2	7:A:801:HOH:O	1.97	0.64
2:B:187:VAL:HG13	2:B:191:GLU:CG	2.28	0.64
2:B:290:LEU:HD11	2:B:308:LEU:HD13	1.79	0.64
2:A:511:GLU:OE2	2:A:546:GLN:HG3	1.98	0.64
2:B:477:LEU:HG	2:B:516:THR:HB	1.80	0.63
2:B:628:ARG:NH2	2:B:628:ARG:HB2	2.13	0.63
2:A:208:GLN:O	2:A:212:GLU:HG3	1.98	0.63
2:B:628:ARG:CB	2:B:628:ARG:HH21	2.12	0.62
2:A:1:MET:N	2:A:5:TYR:HE2	1.98	0.61
1:C:6:DA:H1'	1:C:7:DC:H5"	1.83	0.61
2:B:191:GLU:OE2	2:B:195:ARG:HD3	2.00	0.60
2:B:398:ILE:HG23	2:B:469:ALA:HA	1.82	0.60
1:D:11:DA:H2"	1:D:12:DG:H8	1.63	0.60
2:A:472:THR:HB	2:A:480:GLN:HG3	1.83	0.60
2:A:356:SER:H	2:A:359:GLN:NE2	2.00	0.60
1:D:6:DA:H2"	1:D:7:DC:H5'	1.83	0.60
2:A:443:GLU:O	2:A:447:GLU:HG3	2.02	0.60
2:B:187:VAL:HG13	2:B:191:GLU:HG3	1.83	0.59
2:A:156:PRO:HB2	2:A:175:GLN:HE21	1.66	0.59
2:A:643:GLU:HG2	2:A:645:ARG:CZ	2.33	0.59
2:A:565:LEU:HD22	6:A:701:GOL:H11	1.85	0.59
2:B:445:LEU:HD13	2:B:459:GLN:HB2	1.83	0.59
2:A:287:SER:HB3	2:A:314:ASP:HA	1.85	0.59
1:D:19:DT:H2"	1:D:20:DT:OP1	2.02	0.58
2:B:202:ASN:O	2:B:203:LYS:HD2	2.03	0.58
2:B:226:ASN:C	2:B:226:ASN:HD22	2.06	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:ARG:HG3	2:A:140:ARG:HH11	1.69	0.58
2:B:461:PHE:CZ	2:B:465:ILE:HD11	2.39	0.58
2:A:150:LYS:HZ1	2:A:178:GLN:HE22	1.52	0.57
2:B:472:THR:HG23	2:B:480:GLN:HE21	1.69	0.57
2:A:387:GLU:CD	2:A:505:ARG:HG3	2.24	0.57
2:A:601:VAL:O	2:A:605:ARG:CD	2.53	0.57
2:B:29:ALA:O	2:B:248:ASP:HB2	2.04	0.57
1:D:6:DA:H2"	1:D:7:DC:C5'	2.35	0.57
2:B:326:GLU:CG	2:B:618:ARG:HB2	2.35	0.57
2:A:170:TRP:CE3	2:A:170:TRP:HA	2.40	0.57
2:B:226:ASN:ND2	2:B:229:GLN:H	2.03	0.57
2:A:472:THR:CB	2:A:480:GLN:HG3	2.35	0.56
2:A:601:VAL:O	2:A:605:ARG:HD3	2.05	0.56
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.88	0.56
2:B:637:PRO:HG2	2:B:640:CYS:SG	2.45	0.56
2:A:567:PHE:CE2	6:A:701:GOL:H2	2.40	0.56
2:A:590:GLY:C	2:A:592:LEU:H	2.06	0.56
2:A:140:ARG:HG3	2:A:140:ARG:NH1	2.21	0.56
2:B:47:MET:CE	2:B:54:PRO:HG3	2.36	0.56
2:B:381:ARG:HA	2:B:381:ARG:NE	2.21	0.55
2:B:56:SER:HA	2:B:213:ARG:O	2.06	0.55
2:A:303:ARG:C	2:A:305:GLY:H	2.08	0.55
2:A:47:MET:HE1	2:A:54:PRO:HG3	1.87	0.55
2:A:346:ALA:HB3	2:A:349:GLU:HG3	1.88	0.55
2:B:331:ARG:HH11	2:B:331:ARG:HB3	1.72	0.55
2:B:107:LEU:HD21	2:B:195:ARG:NH1	2.22	0.54
2:B:618:ARG:HD3	7:B:829:HOH:O	2.07	0.54
2:A:288:ASN:HB2	2:A:314:ASP:O	2.07	0.54
2:B:381:ARG:H	2:B:384:GLU:HG3	1.73	0.54
2:A:476:PRO:HD2	2:A:479:VAL:HG11	1.90	0.54
2:A:538:ALA:O	2:A:542:ALA:HB2	2.07	0.54
2:B:124:LYS:HG2	2:B:139:PRO:HG2	1.90	0.54
2:A:503:GLN:O	2:A:507:GLU:HG3	2.08	0.54
2:B:429:THR:OG1	2:B:444:LEU:HD11	2.07	0.54
2:A:156:PRO:HA	2:A:171:GLN:NE2	2.24	0.53
2:A:442:ARG:HD3	2:A:462:MET:HE1	1.91	0.53
2:B:105:ALA:O	2:B:106:ASN:HB3	2.08	0.53
2:B:430:SER:HA	2:B:435:LEU:HD12	1.90	0.53
2:B:346:ALA:HB3	2:B:349:GLU:HG3	1.90	0.53
2:B:43:ILE:HG23	2:B:57:ILE:HD13	1.91	0.53
2:A:61:THR:O	2:A:89:THR:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:VAL:HG23	7:B:905:HOH:O	2.08	0.53
2:B:47:MET:HE1	2:B:54:PRO:HG3	1.90	0.53
2:A:506:ILE:HD12	2:A:509:LEU:HD12	1.91	0.53
2:A:605:ARG:HD2	2:A:605:ARG:N	2.24	0.53
2:B:497:GLU:OE1	2:B:505:ARG:HD2	2.09	0.52
2:A:163:GLY:O	2:A:164:ASN:C	2.48	0.52
2:A:170:TRP:HA	2:A:170:TRP:HE3	1.75	0.52
2:A:222:PHE:O	2:A:225:THR:HG23	2.10	0.52
2:B:421:ARG:HD2	2:B:421:ARG:N	2.24	0.52
2:A:137:TRP:CZ3	2:A:166:VAL:HA	2.45	0.52
2:A:470:GLN:HG3	7:A:919:HOH:O	2.09	0.52
2:B:153:GLY:HA2	2:B:194:LEU:HD13	1.90	0.52
2:B:11:ASN:OD1	2:B:14:GLN:HG3	2.10	0.52
2:B:326:GLU:HG3	2:B:618:ARG:HB2	1.92	0.51
1:D:10:DC:H2"	1:D:11:DA:C5'	2.39	0.51
1:D:10:DC:H2"	1:D:11:DA:H5'	1.92	0.51
2:B:356:SER:H	2:B:359:GLN:NE2	2.08	0.51
2:A:194:LEU:O	2:A:198:GLU:HG3	2.11	0.51
2:A:361:ARG:O	2:A:365:GLU:HG3	2.09	0.51
1:D:18:DG:H21	1:D:19:DT:H71	1.75	0.51
2:A:472:THR:HG22	2:A:475:MET:SD	2.51	0.51
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.25	0.51
2:B:430:SER:HB3	2:B:435:LEU:O	2.09	0.51
2:B:25:LEU:HD12	2:B:275:GLU:O	2.10	0.51
2:B:226:ASN:ND2	2:B:229:GLN:HG3	2.24	0.51
2:A:592:LEU:HD21	7:A:934:HOH:O	2.10	0.51
2:A:592:LEU:HD21	2:A:631:ARG:NH1	2.26	0.50
2:A:375:ARG:CZ	2:A:548:ASP:HB3	2.41	0.50
2:B:61:THR:O	2:B:89:THR:HA	2.11	0.50
2:A:156:PRO:HA	2:A:171:GLN:HE22	1.76	0.50
2:A:102:HIS:NE2	2:A:109:GLN:HB2	2.27	0.50
2:A:389:LYS:HB3	2:A:409:ARG:NE	2.26	0.50
2:A:514:THR:O	2:A:517:ARG:HB3	2.12	0.50
2:A:102:HIS:CE1	2:A:109:GLN:HB2	2.46	0.50
2:A:164:ASN:OD1	2:A:166:VAL:HG23	2.12	0.50
2:B:375:ARG:NE	2:B:548:ASP:HB2	2.27	0.50
2:A:576:GLU:HG3	2:A:579:MET:CG	2.42	0.50
2:B:133:ASP:HB3	2:B:136:GLN:HB3	1.93	0.50
2:A:114:LEU:CD1	2:A:118:ASP:HB3	2.41	0.50
2:A:480:GLN:O	2:A:484:VAL:HG23	2.11	0.50
2:A:500:GLU:O	2:A:504:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:442:ARG:NH1	2:A:462:MET:HE2	2.27	0.49
2:B:37:ARG:HD2	7:B:790:HOH:O	2.11	0.49
2:A:263:ASN:HB2	7:A:721:HOH:O	2.11	0.49
2:A:376:ILE:HG12	2:A:556:LEU:HB2	1.94	0.49
2:B:456:SER:O	2:B:460:ARG:HB2	2.12	0.49
2:B:194:LEU:O	2:B:198:GLU:HG3	2.12	0.49
2:B:394:TYR:O	2:B:398:ILE:HG13	2.13	0.49
2:B:133:ASP:HB3	2:B:136:GLN:CB	2.42	0.49
2:B:381:ARG:HB3	7:B:835:HOH:O	2.12	0.49
2:A:126:LEU:O	2:A:130:MET:HG3	2.13	0.49
2:A:494:TYR:CE2	2:A:505:ARG:HD3	2.47	0.49
2:A:130:MET:O	2:A:131:ASN:HB2	2.13	0.48
2:A:79:GLY:C	2:A:81:SER:H	2.16	0.48
2:B:531:LEU:HD23	2:B:531:LEU:O	2.14	0.48
2:A:401:ARG:HB3	2:A:438:TRP:CD2	2.48	0.48
2:B:31:ALA:HB2	2:B:251:GLN:NE2	2.29	0.48
2:B:435:LEU:HB2	2:B:439:GLN:OE1	2.14	0.48
2:B:498:LYS:C	2:B:500:GLU:H	2.16	0.48
1:D:9:DG:H3'	2:B:421:ARG:HB2	1.95	0.48
1:D:5:DC:P	2:A:124:LYS:HE2	2.54	0.48
1:C:2:DG:H2"	1:C:3:DA:OP2	2.14	0.48
2:B:149:GLN:HG3	2:B:154:LEU:HB2	1.95	0.48
2:A:364:GLU:HG3	2:A:374:TYR:CZ	2.49	0.47
2:A:408:GLU:HG2	2:A:437:LEU:CD1	2.44	0.47
2:B:331:ARG:HH11	2:B:331:ARG:CB	2.27	0.47
2:B:394:TYR:CE1	2:B:410:VAL:HB	2.49	0.47
2:B:447:GLU:O	2:B:448:LYS:C	2.52	0.47
2:B:568:PRO:HA	2:B:607:MET:HB2	1.96	0.47
2:A:588:GLU:CB	2:A:591:ARG:HD2	2.44	0.47
2:B:199:LEU:O	2:B:203:LYS:HB2	2.14	0.47
2:B:476:PRO:HB2	2:B:479:VAL:HG23	1.96	0.47
2:B:628:ARG:NH2	2:B:628:ARG:CB	2.73	0.47
1:D:18:DG:H21	1:D:19:DT:C7	2.27	0.47
1:D:23:DT:H2'	7:B:766:HOH:O	2.12	0.47
1:C:6:DA:H2"	1:C:7:DC:H5'	1.95	0.47
2:A:442:ARG:HH11	2:A:462:MET:HE2	1.78	0.47
2:A:601:VAL:O	2:A:605:ARG:HD2	2.15	0.47
2:B:165:PRO:HG2	2:B:166:VAL:H	1.79	0.47
2:B:380:MET:SD	2:B:384:GLU:HB2	2.54	0.47
2:A:56:SER:HA	2:A:213:ARG:O	2.15	0.47
2:A:476:PRO:O	2:A:479:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:ARG:CG	2:B:454:ALA:N	2.78	0.47
2:B:618:ARG:O	2:B:625:VAL:HG22	2.15	0.47
2:A:481:THR:O	2:A:485:ILE:HG13	2.14	0.47
2:A:1:MET:N	2:A:5:TYR:CE2	2.79	0.47
2:A:564:GLY:H	2:A:605:ARG:HH21	1.59	0.47
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.97	0.47
2:A:60:VAL:HG22	2:A:61:THR:N	2.30	0.47
2:A:150:LYS:NZ	2:A:178:GLN:NE2	2.60	0.47
2:A:290:LEU:HD11	2:A:308:LEU:HD13	1.96	0.47
2:A:27:VAL:HB	2:A:246:VAL:HG12	1.97	0.46
2:B:13:LYS:HG2	2:B:278:ARG:O	2.14	0.46
7:C:596:HOH:O	2:B:619:ARG:HD3	2.14	0.46
2:B:397:LEU:O	2:B:401:ARG:HD2	2.16	0.46
2:B:619:ARG:NH1	2:B:622:GLY:O	2.48	0.46
2:B:155:ARG:O	2:B:157:HIS:N	2.48	0.46
2:A:97:LEU:HD13	7:A:789:HOH:O	2.15	0.46
2:B:429:THR:O	2:B:433:ARG:HG2	2.15	0.46
2:B:480:GLN:O	2:B:484:VAL:HG23	2.15	0.46
2:B:497:GLU:O	2:B:498:LYS:C	2.54	0.46
2:B:110:ASP:OD1	2:B:532:GLN:HG2	2.16	0.46
2:B:290:LEU:HD11	2:B:308:LEU:CD1	2.45	0.46
2:A:282:ASN:HB2	2:A:308:LEU:HD22	1.97	0.46
2:A:308:LEU:HD23	2:A:308:LEU:HA	1.82	0.46
2:B:126:LEU:HG	2:B:130:MET:CE	2.46	0.46
2:A:126:LEU:CD1	2:A:177:TYR:HA	2.46	0.45
2:B:411:VAL:HG13	2:B:412:ASN:N	2.31	0.45
2:B:2:ASP:O	2:B:3:VAL:C	2.54	0.45
2:B:331:ARG:HB3	2:B:331:ARG:NH1	2.31	0.45
2:B:150:LYS:HZ1	2:B:178:GLN:HE22	1.63	0.45
2:B:292:ALA:HB1	2:B:636:LEU:HD22	1.99	0.45
2:B:564:GLY:H	2:B:605:ARG:NH2	2.15	0.45
2:A:494:TYR:O	2:A:497:GLU:HB2	2.17	0.45
1:C:11:DA:H2"	1:C:12:DG:C8	2.51	0.45
2:B:112:GLN:OE1	2:B:396:ARG:HD3	2.17	0.45
2:B:384:GLU:OE2	2:B:542:ALA:HB1	2.16	0.45
1:D:5:DC:H2"	1:D:6:DA:N7	2.29	0.45
2:B:234:ARG:HD3	7:B:903:HOH:O	2.17	0.45
2:A:16:GLU:O	2:A:20:ALA:HB2	2.17	0.44
2:A:459:GLN:HG3	2:A:463:GLU:OE2	2.17	0.44
2:A:475:MET:CE	2:A:479:VAL:HG22	2.47	0.44
2:A:114:LEU:HD12	2:A:118:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:138:PRO:O	2:B:141:GLN:HB2	2.17	0.44
1:D:21:DG:H8	1:D:21:DG:H2'	1.71	0.44
2:A:226:ASN:ND2	2:A:229:GLN:H	2.15	0.44
2:A:411:VAL:HA	2:A:461:PHE:CZ	2.52	0.44
2:A:542:ALA:C	2:A:544:GLU:H	2.21	0.44
1:C:18:DG:H1'	1:C:19:DT:H5'	1.99	0.44
1:D:15:DC:H2"	1:D:16:DT:H72	1.99	0.44
2:A:226:ASN:C	2:A:226:ASN:HD22	2.21	0.44
2:B:271:PHE:HA	2:B:272:PRO:HD3	1.83	0.44
2:B:327:LEU:HD23	2:B:362:VAL:HG13	1.98	0.44
2:A:41:HIS:CD2	2:A:77:LEU:HD22	2.53	0.44
2:A:401:ARG:HH22	2:A:469:ALA:CB	2.29	0.44
1:C:6:DA:H2"	1:C:7:DC:C5'	2.48	0.43
2:A:133:ASP:HB3	2:A:136:GLN:CB	2.48	0.43
2:A:374:TYR:HA	2:A:553:ALA:HB1	2.00	0.43
1:C:12:DG:H2"	1:C:13:DT:OP2	2.19	0.43
1:D:18:DG:C4	2:B:621:TYR:HD2	2.36	0.43
2:B:60:VAL:HG22	2:B:61:THR:N	2.33	0.43
2:B:418:ILE:HD11	2:B:458:LEU:HA	2.00	0.43
2:B:110:ASP:CG	2:B:532:GLN:HE21	2.21	0.43
2:B:446:GLN:HE21	2:B:447:GLU:N	2.17	0.43
2:B:457:ALA:O	2:B:460:ARG:HB3	2.17	0.43
2:B:260:GLN:HG2	7:B:808:HOH:O	2.17	0.43
2:A:398:ILE:HD11	2:A:468:LEU:HB3	2.00	0.43
2:A:156:PRO:CB	2:A:175:GLN:HE21	2.28	0.43
2:B:322:CYS:HB2	2:B:614:TYR:CZ	2.53	0.43
2:A:155:ARG:N	2:A:158:HIS:HD2	1.99	0.43
2:B:10:LEU:HB3	2:B:14:GLN:HB2	2.01	0.43
2:B:155:ARG:CB	2:B:156:PRO:HD2	2.48	0.43
2:B:95:HIS:CD2	2:B:113:ILE:HD11	2.54	0.43
2:B:280:GLU:HG3	7:B:837:HOH:O	2.18	0.43
2:B:202:ASN:C	2:B:203:LYS:HD2	2.38	0.42
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.32	0.42
2:A:79:GLY:C	2:A:81:SER:N	2.72	0.42
2:A:127:ILE:HG23	2:A:132:LEU:HB2	2.02	0.42
2:A:542:ALA:C	2:A:544:GLU:N	2.73	0.42
2:B:467:ALA:O	2:B:471:GLU:HG3	2.19	0.42
2:B:614:TYR:CE2	2:B:629:PRO:HG3	2.53	0.42
2:B:65:LYS:HE2	2:B:377:TYR:CG	2.54	0.42
1:C:20:DT:OP1	2:A:584:MET:HG2	2.20	0.42
2:B:2:ASP:O	2:B:4:SER:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ILE:HD12	2:B:139:PRO:HG3	2.02	0.42
2:B:628:ARG:HH21	2:B:628:ARG:HB3	1.81	0.42
1:C:4:DG:H2"	1:C:5:DC:H5'	2.02	0.42
1:D:6:DA:C1'	1:D:7:DC:H5"	2.46	0.42
2:A:159:ILE:HG13	2:A:171:GLN:NE2	2.34	0.42
2:A:590:GLY:C	2:A:592:LEU:N	2.72	0.42
2:B:590:GLY:HA2	7:B:857:HOH:O	2.20	0.42
1:D:19:DT:OP1	1:D:19:DT:O4'	2.37	0.42
2:A:115:ASP:CG	2:A:389:LYS:HZ1	2.22	0.42
2:B:226:ASN:HB2	7:B:739:HOH:O	2.20	0.42
2:B:639:GLU:CD	2:B:639:GLU:H	2.23	0.42
2:B:155:ARG:C	2:B:157:HIS:H	2.23	0.42
2:A:485:ILE:HG22	2:A:491:ARG:HB2	2.02	0.42
2:B:288:ASN:HD22	2:B:288:ASN:HA	1.70	0.42
2:B:478:HIS:HB3	2:B:517:ARG:HA	2.02	0.42
2:B:556:LEU:HD12	2:B:556:LEU:N	2.35	0.42
2:A:442:ARG:HH11	2:A:462:MET:CE	2.32	0.41
2:B:188:ASP:OD1	2:B:191:GLU:N	2.47	0.41
2:A:137:TRP:CH2	2:A:166:VAL:HA	2.55	0.41
2:A:303:ARG:O	2:A:305:GLY:N	2.52	0.41
2:A:325:ASN:HA	2:A:617:THR:O	2.20	0.41
2:B:273:GLY:O	2:B:275:GLU:HG2	2.20	0.41
2:B:126:LEU:HG	2:B:130:MET:HE1	2.03	0.41
2:B:491:ARG:O	2:B:495:GLU:HG3	2.20	0.41
2:B:4:SER:O	2:B:8:ASP:OD1	2.39	0.41
2:B:200:TRP:CH2	2:B:236:LEU:HG	2.55	0.41
2:A:164:ASN:HB3	2:A:167:GLU:HB3	2.02	0.41
2:A:303:ARG:C	2:A:305:GLY:N	2.73	0.41
2:A:441:CYS:O	2:A:445:LEU:HG	2.21	0.41
2:B:418:ILE:CD1	2:B:458:LEU:HA	2.50	0.41
1:C:15:DC:H2"	1:C:16:DT:OP2	2.21	0.41
1:D:15:DC:C2'	1:D:16:DT:H72	2.51	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:A:203:LYS:CB	2:A:206:ILE:HD12	2.51	0.41
2:A:364:GLU:HG3	2:A:374:TYR:OH	2.20	0.41
2:A:643:GLU:OE1	2:A:645:ARG:NH2	2.54	0.41
2:B:287:SER:HB3	2:B:314:ASP:HA	2.03	0.41
2:B:109:GLN:HG3	2:B:110:ASP:N	2.36	0.41
2:B:117:GLU:OE1	2:B:389:LYS:HE3	2.20	0.41
1:C:18:DG:C1'	1:C:19:DT:H5'	2.51	0.40
2:A:160:GLN:HE21	2:A:160:GLN:HB2	1.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:514:THR:O	2:B:517:ARG:HB3	2.21	0.40
2:B:191:GLU:O	2:B:195:ARG:HB2	2.22	0.40
2:B:203:LYS:HG3	2:B:205:HIS:CE1	2.56	0.40
1:D:10:DC:OP2	2:B:421:ARG:HB2	2.21	0.40
2:A:576:GLU:HG3	2:A:579:MET:HG3	2.03	0.40
2:B:478:HIS:CE1	2:B:479:VAL:HG23	2.56	0.40
2:B:37:ARG:CD	7:B:790:HOH:O	2.69	0.40
2:B:453:ARG:CG	2:B:454:ALA:H	2.34	0.40
2:B:58:MET:HE2	2:B:217:ILE:HG23	2.04	0.40
2:B:397:LEU:HD11	2:B:407:PHE:HA	2.04	0.40

There are no symmetry-related clashes.

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
2	A	650/680 (96%)	610 (94%)	31 (5%)	9 (1%)	11 8
2	B	646/680 (95%)	608 (94%)	26 (4%)	12 (2%)	8 5
All	All	1296/1360 (95%)	1218 (94%)	57 (4%)	21 (2%)	9 7

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	VAL
2	B	158	HIS
2	B	448	LYS
2	B	501	LYS
2	B	589	GLY
2	A	304	LEU
2	A	307	LYS
2	B	307	LYS

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Mol	Chain	Res	Type
2	B	519	PHE
2	A	305	GLY
2	B	156	PRO
2	B	306	LYS
2	B	498	LYS
2	A	454	ALA
2	A	498	LYS
2	B	400	ASN
2	A	2	ASP
2	A	134	GLU
2	A	164	ASN
2	B	157	HIS
2	A	308	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	
2	A	522/574 (91%)	505 (97%)	17 (3%)	38	49
2	B	523/574 (91%)	514 (98%)	9 (2%)	60	74
All	All	1045/1148 (91%)	1019 (98%)	26 (2%)	47	60

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	37	ARG
2	A	103	MET
2	A	160	GLN
2	A	170	TRP
2	A	175	GLN
2	A	195	ARG
2	A	208	GLN
2	A	226	ASN
2	A	235	LEU
2	A	288	ASN

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Mol	Chain	Res	Type
2	A	298	GLU
2	A	308	LEU
2	A	424	ASP
2	A	442	ARG
2	A	483	ARG
2	A	497	GLU
2	A	605	ARG
2	B	37	ARG
2	B	226	ASN
2	B	236	LEU
2	B	288	ASN
2	B	308	LEU
2	B	331	ARG
2	B	381	ARG
2	B	421	ARG
2	B	446	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN
2	A	147	ASN
2	A	158	HIS
2	A	160	GLN
2	A	175	GLN
2	A	178	GLN
2	A	226	ASN
2	A	227	ASN
2	A	265	GLN
2	A	269	ASN
2	A	288	ASN
2	A	359	GLN
2	A	400	ASN
2	A	459	GLN
2	A	496	GLN
2	B	119	GLN
2	B	136	GLN
2	B	147	ASN
2	B	149	GLN
2	B	175	GLN
2	B	178	GLN

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Mol	Chain	Res	Type
2	B	226	ASN
2	B	227	ASN
2	B	288	ASN
2	B	359	GLN
2	B	369	GLN
2	B	446	GLN
2	B	470	GLN
2	B	480	GLN
2	B	503	GLN
2	B	508	ASN
2	B	551	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)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MGF	B	701	5,7,3	0,3,3	-	-	-		
4	MGF	A	699	5,7,3	0,3,3	-	-	-		
6	GOL	A	701	-	5,5,5	0.33	0	5,5,5	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ADP	B	702	4,3	24,29,29	2.82	9 (37%)	29,45,45	2.29	9 (31%)
5	ADP	A	700	4,3	24,29,29	2.87	10 (41%)	29,45,45	2.36	10 (34%)

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
5	ADP	B	702	4,3	-	3/12/32/32	0/3/3/3
6	GOL	A	701	-	-	0/4/4/4	-
5	ADP	A	700	4,3	-	4/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	ADP	C2-N1	6.04	1.45	1.33
5	B	702	ADP	C2-N3	6.00	1.41	1.32
5	B	702	ADP	C2-N1	5.85	1.44	1.33
5	A	700	ADP	C2-N3	5.77	1.41	1.32
5	B	702	ADP	C4-N3	5.36	1.43	1.35
5	A	700	ADP	C4-N3	5.27	1.42	1.35
5	A	700	ADP	C2'-C1'	-5.27	1.45	1.53
5	A	700	ADP	C5-C4	4.90	1.53	1.40
5	B	702	ADP	C2'-C1'	-4.90	1.46	1.53
5	B	702	ADP	C5-C4	4.49	1.52	1.40
5	B	702	ADP	C6-C5	3.18	1.55	1.43
5	A	700	ADP	C6-C5	3.07	1.54	1.43
5	A	700	ADP	C3'-C4'	-2.87	1.45	1.53
5	B	702	ADP	PB-O3B	2.87	1.65	1.54
5	A	700	ADP	PB-O3B	2.83	1.65	1.54
5	A	700	ADP	PB-O2B	-2.83	1.44	1.54
5	B	702	ADP	PB-O2B	-2.73	1.44	1.54
5	B	702	ADP	C3'-C4'	-2.34	1.47	1.53
5	A	700	ADP	C5-N7	-2.03	1.32	1.39

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	702	ADP	N3-C2-N1	-5.27	120.45	128.68
5	A	700	ADP	N3-C2-N1	-5.13	120.66	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	700	ADP	N6-C6-N1	5.07	129.09	118.57
5	A	700	ADP	C2-N1-C6	4.89	127.12	118.75
5	B	702	ADP	N6-C6-N1	4.89	128.72	118.57
5	B	702	ADP	C2-N1-C6	4.69	126.78	118.75
5	B	702	ADP	C1'-N9-C4	-3.29	120.86	126.64
5	A	700	ADP	C5-C6-N1	-3.23	113.04	120.35
5	A	700	ADP	C1'-N9-C4	-3.19	121.03	126.64
5	A	700	ADP	O5'-PA-O1A	3.15	121.37	109.07
5	B	702	ADP	C4-C5-N7	-3.04	106.23	109.40
5	A	700	ADP	O2A-PA-O1A	-3.04	97.21	112.24
5	B	702	ADP	C5-C6-N1	-3.03	113.48	120.35
5	A	700	ADP	C4-C5-N7	-3.01	106.26	109.40
5	B	702	ADP	O5'-PA-O1A	2.81	120.04	109.07
5	B	702	ADP	O2A-PA-O1A	-2.79	98.45	112.24
5	B	702	ADP	O4'-C1'-C2'	-2.64	103.07	106.93
5	A	700	ADP	O4'-C1'-C2'	-2.64	103.08	106.93
5	A	700	ADP	O2B-PB-O1B	2.03	118.64	110.68

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	700	ADP	PA-O3A-PB-O1B
5	B	702	ADP	PA-O3A-PB-O1B
5	A	700	ADP	PA-O3A-PB-O2B
5	B	702	ADP	PA-O3A-PB-O2B
5	A	700	ADP	C5'-O5'-PA-O3A
5	A	700	ADP	C5'-O5'-PA-O1A
5	B	702	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

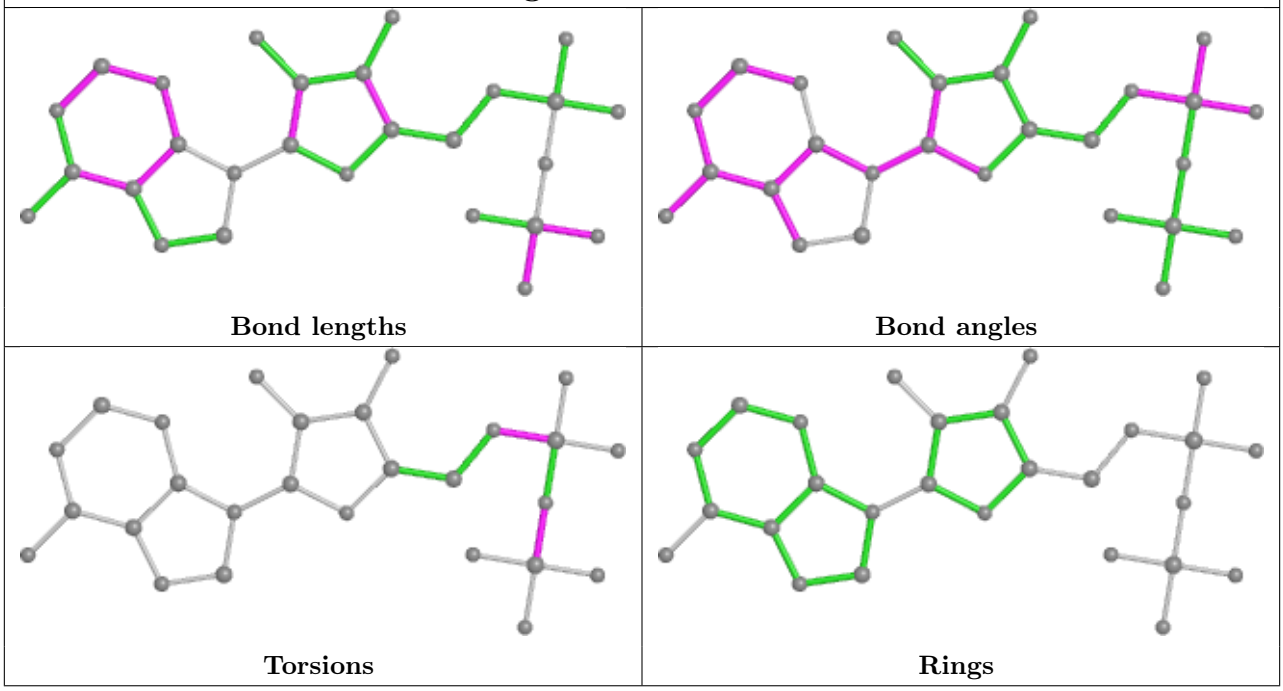
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	701	GOL	2	0

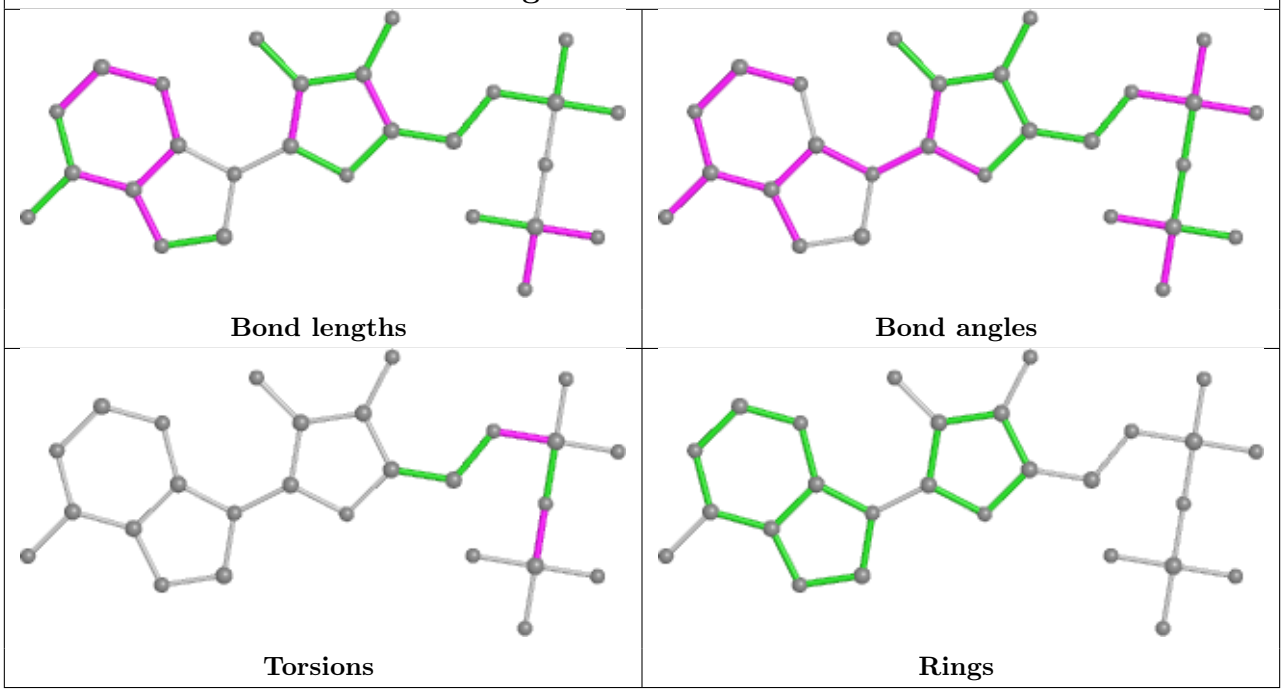
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ADP A 700



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^{th} 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	C	23/25 (92%)	0.42	1 (4%)	35	33	35, 83, 122, 136	0
1	D	23/25 (92%)	0.52	1 (4%)	35	33	38, 82, 108, 113	0
2	A	654/680 (96%)	0.24	39 (5%)	21	20	25, 49, 85, 104	1 (0%)
2	B	652/680 (95%)	0.25	41 (6%)	20	19	26, 54, 94, 106	0
All	All	1352/1410 (95%)	0.25	82 (6%)	21	20	25, 52, 92, 136	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	499	GLY	6.8
2	A	590	GLY	6.8
2	B	304	LEU	6.6
2	B	159	ILE	6.3
2	A	499	GLY	5.4
2	A	526	GLU	5.1
2	A	648	ALA	5.0
2	A	649	THR	4.9
2	A	166	VAL	4.7
2	A	81	SER	4.7
2	A	496	GLN	4.5
2	A	304	LEU	4.5
2	B	445	LEU	4.5
2	B	450	LEU	4.4
2	B	654	VAL	4.3
2	A	305	GLY	4.3
2	B	137	TRP	4.3
2	A	651	SER	4.2
2	B	158	HIS	4.1
2	A	500	GLU	4.1
2	B	305	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	302	GLY	4.0
2	B	446	GLN	3.8
2	A	523	GLU	3.7
2	B	81	SER	3.7
2	A	547	ALA	3.5
2	B	80	THR	3.5
2	A	5	TYR	3.5
2	B	144	TRP	3.4
2	B	82	GLN	3.4
2	B	550	TRP	3.4
2	A	650	VAL	3.3
2	B	500	GLU	3.3
2	B	165	PRO	3.3
2	B	131	ASN	3.2
2	B	130	MET	3.2
2	A	656	HIS	3.1
2	B	460	ARG	3.1
2	B	503	GLN	3.0
1	D	19	DT	3.0
2	A	497	GLU	3.0
2	B	459	GLN	3.0
2	A	165	PRO	3.0
2	A	543	GLY	2.9
2	A	502	GLY	2.9
2	B	156	PRO	2.8
2	A	82	GLN	2.7
2	A	302	GLY	2.7
2	B	470	GLN	2.7
2	A	137	TRP	2.6
2	A	647	ARG	2.6
2	B	472	THR	2.5
2	A	1	MET	2.5
2	B	502	GLY	2.5
2	B	476	PRO	2.5
2	A	527	ASP	2.5
2	A	80	THR	2.4
2	A	495	GLU	2.4
2	B	520	SER	2.3
2	A	504	THR	2.3
2	A	503	GLN	2.3
2	B	441	CYS	2.3
2	A	164	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	63	THR	2.2
2	B	114	LEU	2.2
2	A	501	LYS	2.2
2	B	498	LYS	2.2
2	A	558	THR	2.2
2	A	134	GLU	2.2
2	B	496	GLN	2.2
2	A	376	ILE	2.2
1	C	1	DC	2.1
2	B	280	GLU	2.1
2	B	526	GLU	2.1
2	B	135	LYS	2.1
2	B	3	VAL	2.1
2	A	460	ARG	2.1
2	B	164	ASN	2.1
2	B	474	ASP	2.1
2	A	163	GLY	2.0
2	B	471	GLU	2.0
2	B	458	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^{th} 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
6	GOL	A	701	6/6	0.67	0.28	65,68,69,69	0
3	MG	B	681	1/1	0.96	0.11	33,33,33,33	0
3	MG	A	681	1/1	0.96	0.22	36,36,36,36	0
4	MGF	A	699	4/4	0.97	0.14	33,33,35,35	0

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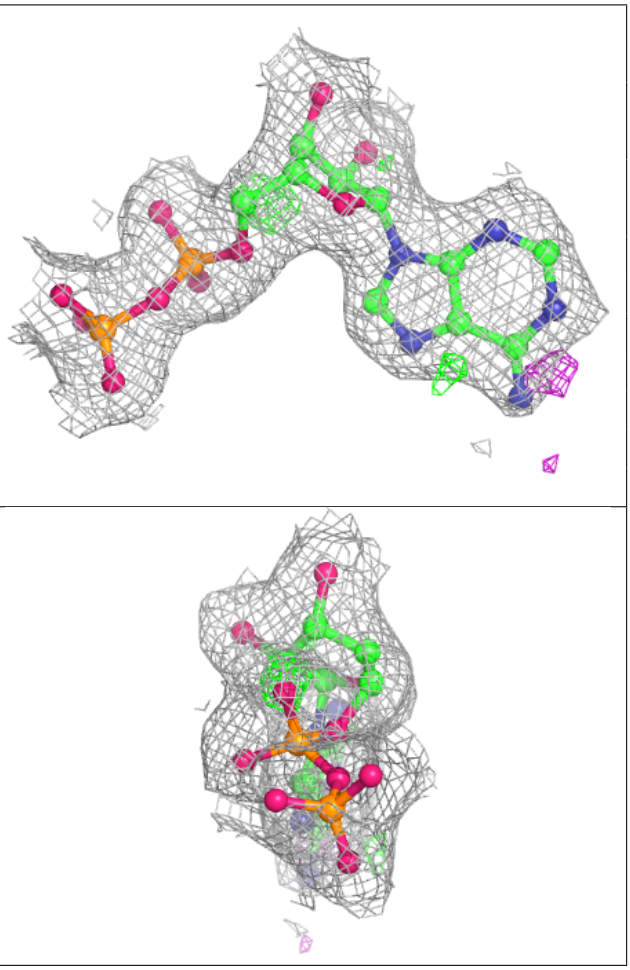
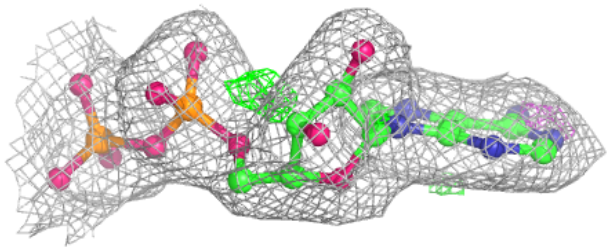
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ADP	A	700	27/27	0.98	0.13	29,36,43,45	0
5	ADP	B	702	27/27	0.98	0.12	29,34,43,44	0
4	MGF	B	701	4/4	0.98	0.11	29,31,34,36	0

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 700:

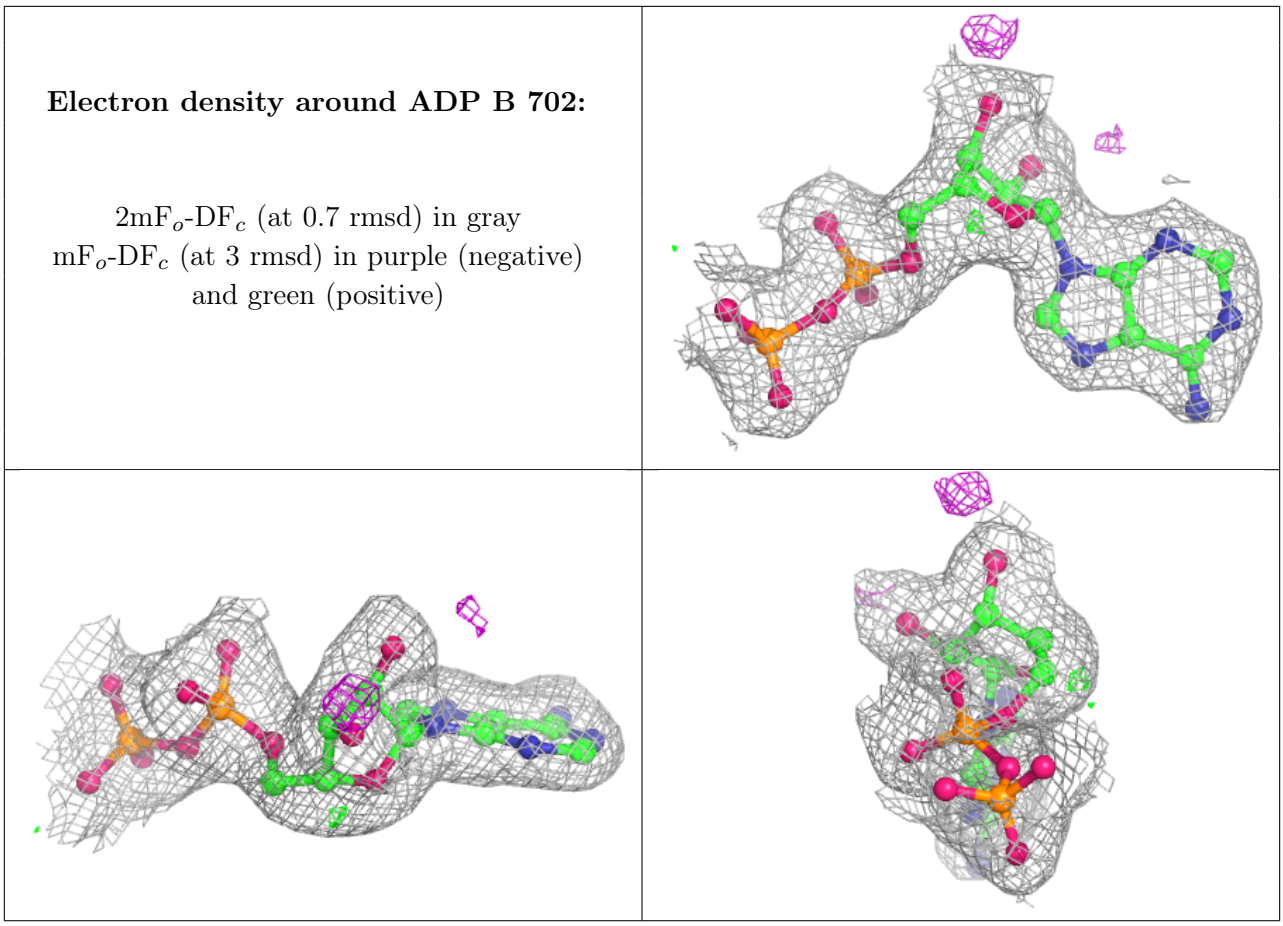
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





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)



6.5 Other polymers (i)

There are no such residues in this entry.