Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 12:43 am GMT

PDB ID	:	4C2U
Title	:	Crystal structure of Deinococcus radiodurans UvrD in complex with DNA, Form 1
Authors	:	Stelter, M.; Acajjaoui, S.; McSweeney, S.; Timmins, J.
Deposited on	:	2013-08-20
Resolution	:	2.55 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 ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

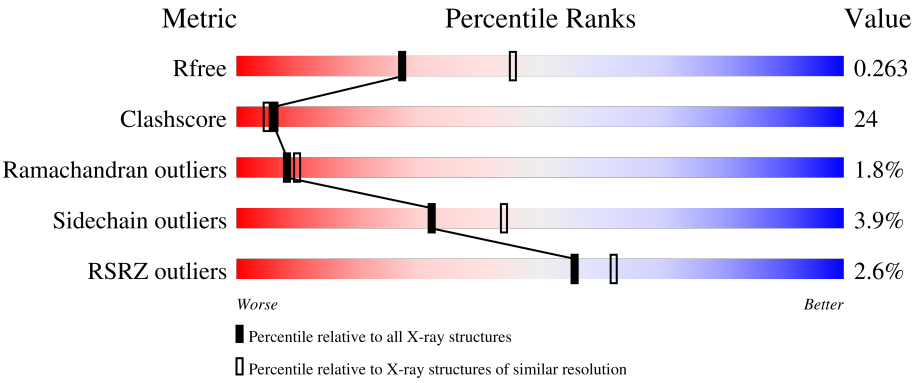
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	665	3% 69% 26%
1	D	665	3% 66% 29%
2	X	25	4% 8% 56% 32%
3	Y	25	4% 52% 36% 8%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11697 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 DNA HELICASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	658	Total	C	N	O	S	0	7	0
			5227	3266	953	993	15			
1	D	658	Total	C	N	O	S	0	7	0
			5234	3272	953	994	15			

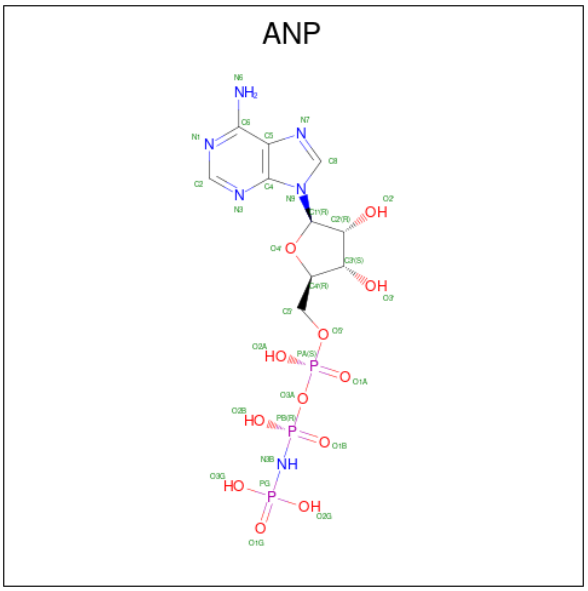
- Molecule 2 is a DNA chain called REV25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	24	Total	C	N	O	P	0	0	0
			487	233	82	148	24			

- Molecule 3 is a DNA chain called FOR25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	23	Total	C	N	O	P	0	0	0
			469	225	75	146	23			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).

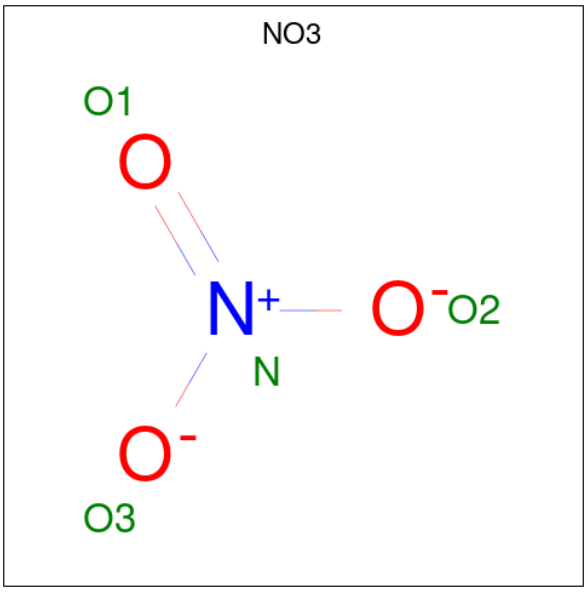


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

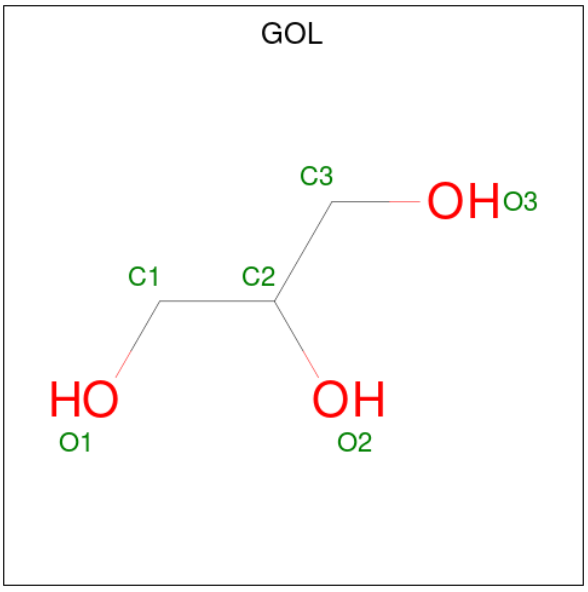
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N O 4 1 3	0	0
6	A	1	Total N O 4 1 3	0	0
6	D	1	Total N O 4 1 3	0	0
6	D	1	Total N O 4 1 3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	D	1	Total Na 1 1	0	0

- Molecule 9 is water.

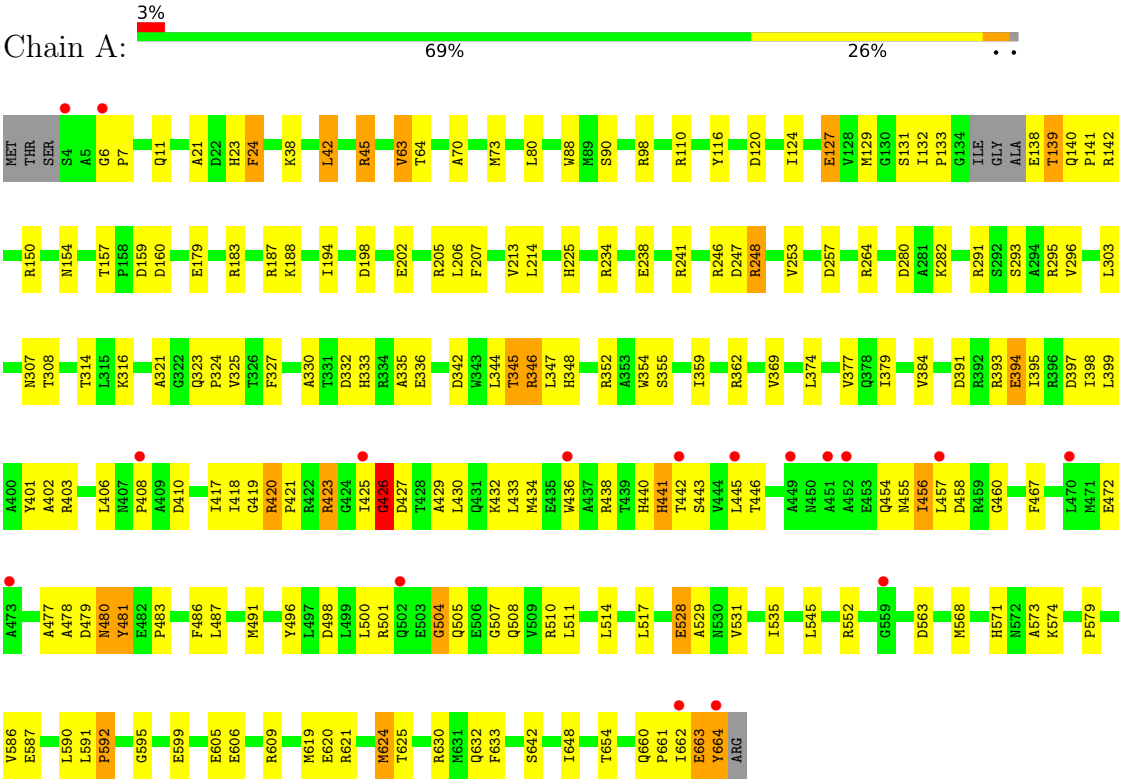
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	85	Total O 85 85	0	0
9	D	95	Total O 95 95	0	0
9	X	3	Total O 3 3	0	0
9	Y	3	Total O 3 3	0	0

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.

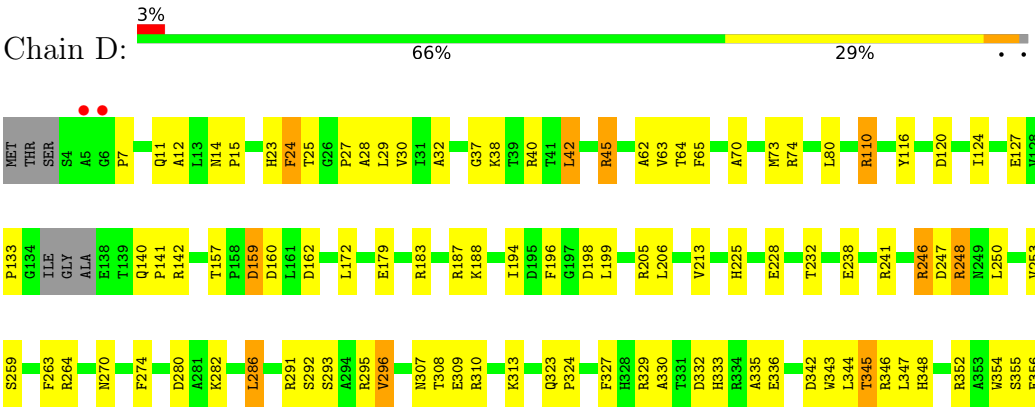
• Molecule 1: DNA HELICASE II

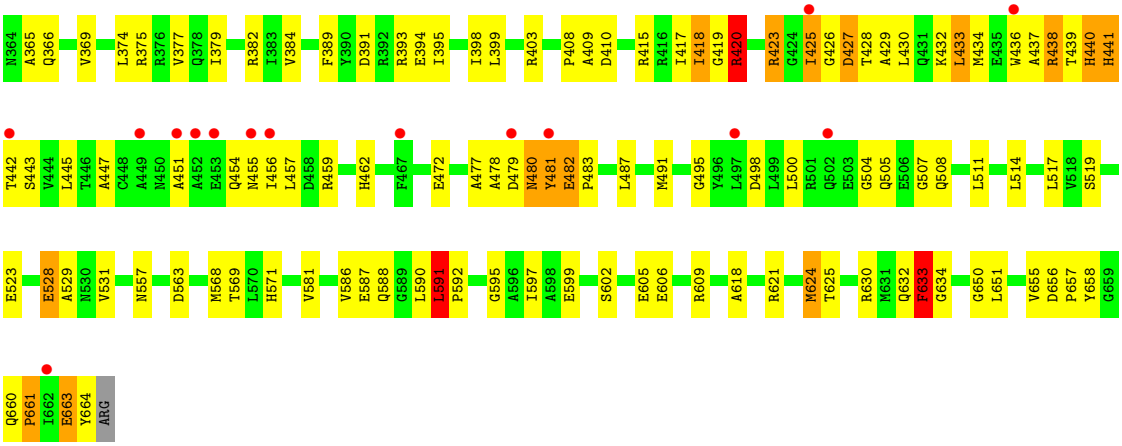
Chain A:



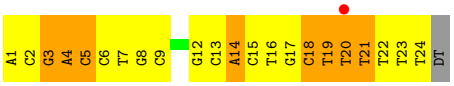
• Molecule 1: DNA HELICASE II

Chain D:

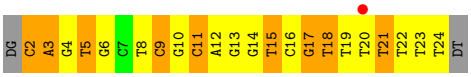




• Molecule 2: REV25



• Molecule 3: FOR25



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.57Å 67.45Å 386.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.55 47.74 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.74-2.55) 99.5 (47.74-2.55)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.84 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.6.0085	Depositor
R, R_{free}	0.211 , 0.267 0.210 , 0.263	Depositor DCC
R_{free} test set	2971 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.2	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.487 for k,h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11697	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: GOL, NA, ANP, NO3, MG

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	0.82	2/5330 (0.0%)	0.83	5/7207 (0.1%)
1	D	0.82	1/5335 (0.0%)	0.84	5/7213 (0.1%)
2	X	1.00	0/543	1.98	27/835 (3.2%)
3	Y	1.59	4/522 (0.8%)	2.24	21/804 (2.6%)
All	All	0.88	7/11730 (0.1%)	1.04	58/16059 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	D	0	3
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	Y	15	DT	C4'-O4'	19.55	1.64	1.45
3	Y	2	DC	O3'-P	-12.75	1.45	1.61
3	Y	17	DG	C4'-O4'	11.79	1.56	1.45
3	Y	17	DG	O3'-P	8.57	1.71	1.61
1	A	63	VAL	CB-CG1	6.07	1.65	1.52
1	D	63	VAL	CB-CG1	6.04	1.65	1.52
1	A	45	ARG	CG-CD	-5.01	1.39	1.51

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Y	15	DT	C1'-O4'-C4'	-20.96	89.14	110.10
3	Y	15	DT	O4'-C4'-C3'	-15.44	96.73	106.00
3	Y	21	DT	O4'-C1'-N1	-12.63	99.16	108.00
2	X	21	DT	O4'-C1'-N1	-12.59	99.19	108.00
3	Y	15	DT	C5'-C4'-O4'	-11.05	88.30	109.30
3	Y	5	DT	C5'-C4'-O4'	-10.69	89.00	109.30
3	Y	17	DG	O4'-C4'-C3'	-10.39	99.76	106.00
2	X	9	DC	O4'-C1'-N1	10.28	115.20	108.00
2	X	14	DA	C1'-O4'-C4'	-9.61	100.49	110.10
3	Y	5	DT	C1'-O4'-C4'	-9.34	100.76	110.10
2	X	21	DT	OP2-P-O3'	8.79	124.54	105.20
1	D	248	ARG	NE-CZ-NH1	7.44	124.02	120.30
2	X	24	DT	C5-C4-O4	-7.39	119.72	124.90
3	Y	5	DT	O4'-C1'-N1	7.27	113.09	108.00
1	A	248	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	D	248	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	248	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	Y	2	DC	P-O3'-C3'	6.79	127.85	119.70
2	X	18	DC	P-O3'-C3'	6.77	127.83	119.70
3	Y	21	DT	C6-C5-C7	-6.72	118.87	122.90
1	A	426	GLY	O-C-N	-6.67	112.02	122.70
3	Y	15	DT	C5-C4-O4	-6.67	120.23	124.90
2	X	4	DA	N1-C6-N6	6.64	122.59	118.60
2	X	21	DT	C5-C6-N1	-6.55	119.77	123.70
2	X	14	DA	N1-C6-N6	6.50	122.50	118.60
3	Y	18	DT	O4'-C1'-N1	6.49	112.54	108.00
2	X	19	DT	P-O3'-C3'	6.44	127.43	119.70
3	Y	9	DC	O4'-C1'-N1	6.33	112.43	108.00
2	X	20	DT	O3'-P-O5'	-6.31	92.00	104.00
3	Y	23	DT	C5-C4-O4	-6.27	120.51	124.90
1	A	159	ASP	CB-CG-OD1	6.12	123.81	118.30
3	Y	3	DA	N1-C6-N6	6.03	122.22	118.60
2	X	23	DT	N3-C2-O2	5.97	125.88	122.30
2	X	9	DC	N1-C2-O2	5.91	122.44	118.90
2	X	23	DT	O4'-C1'-C2'	5.85	110.58	105.90
2	X	21	DT	N1-C2-O2	-5.84	118.43	123.10
2	X	14	DA	C5-C6-N6	-5.83	119.03	123.70
2	X	23	DT	C6-N1-C2	5.82	124.21	121.30
2	X	14	DA	N9-C4-C5	-5.61	103.56	105.80
2	X	21	DT	C2-N3-C4	-5.60	123.84	127.20
1	D	159	ASP	CB-CG-OD1	5.56	123.31	118.30
2	X	23	DT	N3-C4-C5	5.54	118.53	115.20
2	X	3	DG	C3'-C2'-C1'	-5.54	95.86	102.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	23	DT	C5-C4-O4	-5.50	121.05	124.90
2	X	21	DT	C6-C5-C7	-5.48	119.61	122.90
2	X	24	DT	N3-C4-O4	5.46	123.18	119.90
3	Y	11	DC	N1-C2-O2	5.40	122.14	118.90
2	X	5	DC	O4'-C1'-N1	5.38	111.76	108.00
3	Y	23	DT	N3-C4-C5	5.30	118.38	115.20
3	Y	23	DT	N3-C2-O2	5.26	125.45	122.30
2	X	3	DG	C5-C6-O6	-5.25	125.45	128.60
1	A	426	GLY	CA-C-N	5.22	128.68	117.20
1	D	246	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	Y	8	DT	C1'-O4'-C4'	-5.18	104.92	110.10
3	Y	21	DT	C4'-C3'-O3'	-5.16	96.79	109.70
3	Y	24	DT	C5-C4-O4	-5.16	121.29	124.90
1	D	591	LEU	C-N-CD	-5.13	109.30	120.60
2	X	21	DT	OP1-P-O3'	-5.06	94.07	105.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	420	ARG	Peptide
1	A	591	LEU	Mainchain,Peptide
1	D	420	ARG	Sidechain
1	D	591	LEU	Mainchain,Peptide

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	5227	0	5159	209	0
1	D	5234	0	5160	249	0
2	X	487	0	273	61	0
3	Y	469	0	264	51	0
4	A	31	0	13	1	0
4	D	31	0	13	3	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	8	0	0	0	0
6	D	8	0	0	0	0
7	A	6	0	8	1	0
7	D	6	0	8	1	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	A	85	0	0	3	0
9	D	95	0	0	10	0
9	X	3	0	0	1	0
9	Y	3	0	0	0	0
All	All	11697	0	10898	540	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 24.

All (540) 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)
3:Y:15:DT:O4'	3:Y:15:DT:C4'	1.64	1.25
1:A:491:MET:HE1	1:A:514:LEU:HB3	1.25	1.17
3:Y:20:DT:H1'	3:Y:21:DT:H5"	1.23	1.16
1:A:660:GLN:HB2	1:A:661:PRO:CD	1.76	1.15
2:X:14:DA:N6	3:Y:5:DT:H3	1.43	1.14
1:D:430:LEU:HA	1:D:433:LEU:HD12	1.27	1.13
1:A:346:ARG:HG3	1:A:346:ARG:HH11	1.13	1.10
1:A:454:GLN:HG3	1:A:455:ASN:H	1.14	1.10
1:D:116:TYR:CE2	1:D:124:ILE:HD11	1.86	1.10
1:A:426:GLY:HA3	1:A:429:ALA:HB3	1.23	1.09
1:D:393:ARG:HH22	1:D:420:ARG:NH2	1.52	1.07
1:D:454:GLN:HG3	1:D:455:ASN:H	0.98	1.07
1:D:426:GLY:CA	1:D:429:ALA:HB3	1.84	1.07
1:A:116:TYR:CE2	1:A:124:ILE:HD11	1.89	1.07
1:D:491:MET:CE	1:D:514:LEU:HB3	1.85	1.06
2:X:4:DA:H1'	2:X:5:DC:OP2	1.55	1.04
2:X:16:DT:H2"	2:X:17:DG:OP2	1.52	1.04
1:D:454:GLN:HG3	1:D:455:ASN:N	1.71	1.03
1:A:138:GLU:HG3	1:A:139:THR:H	1.24	1.03
1:D:481[B]:TYR:O	1:D:481[B]:TYR:CD1	2.12	1.02
1:D:426:GLY:HA3	1:D:429:ALA:CB	1.90	1.01
1:A:346:ARG:HH11	1:A:346:ARG:CG	1.75	0.99
1:D:426:GLY:HA3	1:D:429:ALA:HB3	1.00	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:GLY:HA2	1:D:425:ILE:HG13	1.42	0.98
2:X:18:DC:H1'	2:X:19:DT:H5"	1.45	0.98
3:Y:20:DT:H1'	3:Y:21:DT:C5'	1.92	0.98
1:D:480:ASN:O	1:D:481[B]:TYR:HB2	1.60	0.97
1:A:131:SER:HB2	1:A:183:ARG:HH22	1.30	0.96
1:D:480:ASN:O	1:D:481[B]:TYR:CB	2.13	0.96
1:D:393:ARG:NH2	1:D:420:ARG:HH22	1.63	0.95
1:A:487:LEU:O	1:A:491:MET:HG3	1.66	0.95
1:A:131:SER:HB2	1:A:183:ARG:NH2	1.82	0.95
1:D:481[B]:TYR:O	1:D:481[B]:TYR:HD1	1.45	0.94
1:A:660:GLN:HB2	1:A:661:PRO:HD3	1.47	0.94
2:X:2:DC:OP2	2:X:2:DC:H6	1.49	0.94
1:D:425:ILE:HD13	1:D:425:ILE:N	1.83	0.94
2:X:15:DC:H42	3:Y:4:DG:H1	1.11	0.93
1:A:342:ASP:CG	1:A:346:ARG:HH12	1.72	0.92
1:A:660:GLN:HB2	1:A:661:PRO:HD2	1.51	0.92
1:D:491:MET:HE2	1:D:514:LEU:HD13	1.51	0.92
1:A:432:LYS:HZ2	1:A:457:LEU:HA	1.33	0.92
1:D:393:ARG:HH22	1:D:420:ARG:HH22	0.93	0.92
1:A:348:HIS:CE1	1:A:354:TRP:CE2	2.57	0.91
1:D:491:MET:HE1	1:D:514:LEU:HB3	1.53	0.91
2:X:2:DC:C2	3:Y:17:DG:N2	2.39	0.90
1:A:116:TYR:HE2	1:A:124:ILE:HD11	1.37	0.90
1:D:116:TYR:HE2	1:D:124:ILE:HD11	1.33	0.90
1:A:354:TRP:CZ3	1:A:379:ILE:HG23	2.06	0.89
3:Y:15:DT:O4'	3:Y:15:DT:C5'	2.20	0.89
1:A:391:ASP:OD1	7:A:1668:GOL:H2	1.74	0.88
1:A:660:GLN:CB	1:A:661:PRO:CD	2.53	0.87
1:D:454:GLN:CG	1:D:455:ASN:H	1.86	0.87
1:A:454:GLN:HG3	1:A:455:ASN:N	1.88	0.87
1:D:393:ARG:NH2	1:D:420:ARG:HH12	1.72	0.86
1:A:432:LYS:NZ	1:A:457:LEU:HA	1.90	0.86
1:D:430:LEU:HA	1:D:433:LEU:CD1	2.04	0.86
1:A:138:GLU:HG3	1:A:139:THR:N	1.90	0.86
1:D:433:LEU:HG	1:D:457:LEU:HD11	1.57	0.85
1:A:487:LEU:HD13	1:A:517:LEU:CD2	2.06	0.84
2:X:17:DG:OP2	2:X:17:DG:C8	2.30	0.84
1:D:423:ARG:H	1:D:425:ILE:CD1	1.91	0.84
1:A:308:THR:HA	9:A:2052:HOH:O	1.76	0.84
1:A:491:MET:CE	1:A:514:LEU:HB3	2.06	0.84
1:D:391:ASP:OD1	7:D:1668:GOL:H2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:430:LEU:CA	1:D:433:LEU:HD12	2.08	0.83
2:X:15:DC:N4	3:Y:4:DG:H1	1.75	0.83
1:D:663:GLU:O	1:D:664:TYR:HD1	1.61	0.83
2:X:18:DC:C5	2:X:19:DT:H72	2.14	0.83
1:D:440:HIS:O	1:D:441:HIS:HB2	1.78	0.83
3:Y:17:DG:H2"	3:Y:18:DT:O5'	1.78	0.82
1:A:188:LYS:HE3	1:A:198:ASP:OD2	1.79	0.82
1:D:487:LEU:HD13	1:D:517:LEU:CD2	2.10	0.81
1:D:519:SER:O	1:D:523:GLU:HG3	1.81	0.81
1:D:131:SER:HB2	1:D:183:ARG:NH2	1.96	0.80
1:D:491:MET:HE3	1:D:514:LEU:HB3	1.64	0.80
1:D:398:ILE:HD12	1:D:491:MET:HG2	1.62	0.80
1:A:454:GLN:CG	1:A:455:ASN:H	1.90	0.80
2:X:16:DT:C2'	2:X:17:DG:OP2	2.30	0.80
1:D:454:GLN:O	1:D:456:ILE:HG13	1.82	0.79
1:A:479:ASP:C	1:A:480:ASN:HD22	1.85	0.79
1:A:663:GLU:O	1:A:664:TYR:HB2	1.83	0.78
1:D:436:TRP:CZ2	1:D:440:HIS:CD2	2.72	0.78
1:D:663:GLU:O	1:D:664:TYR:CD1	2.37	0.78
3:Y:20:DT:H2"	3:Y:21:DT:OP2	1.83	0.78
1:A:7:PRO:HB3	1:A:80:LEU:HD22	1.65	0.77
1:A:479:ASP:O	1:A:480:ASN:ND2	2.16	0.77
1:D:426:GLY:O	1:D:430:LEU:HB3	1.84	0.77
1:D:393:ARG:HH22	1:D:420:ARG:CZ	1.98	0.77
1:D:425:ILE:HD13	1:D:425:ILE:H	1.50	0.77
1:D:425:ILE:N	1:D:425:ILE:CD1	2.47	0.77
2:X:2:DC:OP2	2:X:2:DC:C6	2.37	0.76
1:D:459:ARG:HD2	3:Y:9:DC:H4'	1.67	0.76
1:A:354:TRP:CH2	1:A:379:ILE:HG23	2.20	0.75
1:A:477:ALA:HA	1:A:481:TYR:CE2	2.21	0.75
1:D:116:TYR:CE2	1:D:124:ILE:CD1	2.67	0.75
1:A:138:GLU:CG	1:A:139:THR:H	1.99	0.75
3:Y:3:DA:H8	3:Y:3:DA:OP2	1.68	0.75
1:D:480:ASN:O	1:D:481[A]:TYR:CD2	2.41	0.74
1:D:480:ASN:O	1:D:481[A]:TYR:HD2	1.71	0.74
3:Y:12:DA:H2"	3:Y:13:DG:C8	2.22	0.74
1:A:660:GLN:CB	1:A:661:PRO:HD2	2.16	0.74
1:D:323:GLN:OE1	1:D:621:ARG:HD2	1.87	0.74
1:A:38:LYS:HB3	1:A:253:VAL:HG11	1.68	0.74
1:D:348:HIS:ND1	1:D:354:TRP:CZ2	2.56	0.73
1:A:348:HIS:HE1	1:A:354:TRP:CE2	2.05	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:HIS:ND1	1:A:354:TRP:CZ2	2.57	0.73
1:D:7:PRO:HB3	1:D:80:LEU:HD22	1.71	0.72
1:D:632:GLN:HG3	1:D:633:PHE:H	1.52	0.72
1:A:323:GLN:OE1	1:A:621:ARG:HD2	1.89	0.72
1:D:487:LEU:O	1:D:491:MET:HG3	1.88	0.72
1:A:348:HIS:CE1	1:A:354:TRP:CZ2	2.77	0.72
1:D:430:LEU:O	1:D:434:MET:HG3	1.88	0.72
1:D:188:LYS:HE3	1:D:198:ASP:OD2	1.90	0.72
1:D:131:SER:HB2	1:D:183:ARG:HH22	1.55	0.72
1:A:206:LEU:HD21	1:A:213:VAL:HG11	1.72	0.71
1:A:346:ARG:HG3	1:A:346:ARG:NH1	1.93	0.71
1:D:403:ARG:NH1	1:D:410:ASP:OD2	2.23	0.71
1:D:487:LEU:HD13	1:D:517:LEU:HD21	1.72	0.71
1:A:347:LEU:HB3	1:A:352[B]:ARG:HH21	1.56	0.70
1:D:587:GLU:OE1	1:D:630:ARG:NH1	2.24	0.70
1:A:587:GLU:OE1	1:A:630:ARG:NH1	2.24	0.70
1:D:423:ARG:H	1:D:425:ILE:HD11	1.54	0.70
1:A:342:ASP:CG	1:A:346:ARG:NH1	2.44	0.70
1:A:487:LEU:HD13	1:A:517:LEU:HD21	1.73	0.70
1:A:345:THR:O	1:A:346:ARG:C	2.30	0.70
2:X:3:DG:H2"	2:X:4:DA:C8	2.27	0.70
1:D:393:ARG:NH2	1:D:420:ARG:NH1	2.41	0.69
2:X:18:DC:C4	2:X:19:DT:H72	2.28	0.69
1:A:42:LEU:HD13	1:A:253:VAL:HG21	1.75	0.69
3:Y:16:DC:H2"	3:Y:17:DG:OP2	1.91	0.69
1:D:491:MET:CE	1:D:514:LEU:HD13	2.22	0.69
1:D:451:ALA:O	1:D:456:ILE:HG23	1.92	0.69
1:A:355:SER:HB3	1:A:563:ASP:HA	1.75	0.69
1:A:38:LYS:HB3	1:A:253:VAL:CG1	2.23	0.68
1:A:188:LYS:HE2	1:A:194:ILE:HA	1.73	0.68
2:X:5:DC:H42	3:Y:14:DG:H1	1.39	0.68
1:D:529:ALA:HB1	9:D:2086:HOH:O	1.92	0.68
1:D:355:SER:HB3	1:D:563:ASP:HA	1.75	0.68
1:A:419:GLY:HA2	1:A:425:ILE:HG13	1.76	0.67
2:X:15:DC:C5	2:X:16:DT:C4	2.82	0.67
1:D:188:LYS:HE2	1:D:194:ILE:HA	1.75	0.67
1:A:187:ARG:NH2	1:A:438:ARG:HH21	1.92	0.67
2:X:21:DT:H2"	2:X:22:DT:O5'	1.94	0.67
1:D:409:ALA:HB3	9:D:2080:HOH:O	1.93	0.67
3:Y:15:DT:O4'	3:Y:15:DT:O5'	2.13	0.67
1:D:660:GLN:OE1	1:D:660:GLN:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:TRP:CZ3	1:D:379:ILE:HG23	2.30	0.67
1:D:423:ARG:N	1:D:425:ILE:HD11	2.09	0.67
1:D:606:GLU:OE1	1:D:609:ARG:NH1	2.28	0.66
1:D:232:THR:HG23	1:D:270:ASN:OD1	1.94	0.66
2:X:5:DC:N3	3:Y:14:DG:N2	2.39	0.66
1:D:110[B]:ARG:HH11	1:D:110[B]:ARG:HB2	1.60	0.66
1:D:432:LYS:HB3	1:D:457:LEU:HD22	1.78	0.66
1:D:440:HIS:O	1:D:441:HIS:CB	2.43	0.66
1:D:342:ASP:OD2	1:D:346:ARG:NH2	2.30	0.66
1:D:480:ASN:O	1:D:481[A]:TYR:HB2	1.96	0.66
1:A:377:VAL:HG12	1:A:377:VAL:O	1.96	0.65
3:Y:21:DT:H2"	3:Y:22:DT:O5'	1.97	0.65
1:A:662:ILE:HG22	1:A:662:ILE:O	1.95	0.65
1:D:308:THR:HA	9:D:2061:HOH:O	1.95	0.65
1:D:462:HIS:HB2	9:D:2083:HOH:O	1.96	0.65
1:D:395:ILE:HG23	1:D:517:LEU:HD12	1.77	0.65
1:A:342:ASP:OD2	1:A:346:ARG:NH1	2.29	0.65
1:D:342:ASP:OD2	1:D:346:ARG:NE	2.30	0.65
1:D:423:ARG:H	1:D:425:ILE:HD13	1.59	0.65
1:A:342:ASP:OD2	1:A:346:ARG:NH2	2.29	0.65
1:A:342:ASP:OD2	1:A:346:ARG:CZ	2.45	0.65
1:A:354:TRP:CZ3	1:A:379:ILE:CG2	2.79	0.65
1:A:480:ASN:HB2	1:A:481:TYR:CE1	2.32	0.65
1:D:437:ALA:O	1:D:441:HIS:N	2.30	0.65
1:A:332:ASP:HB3	1:A:335:ALA:H	1.61	0.64
1:A:346:ARG:CG	1:A:346:ARG:NH1	2.47	0.64
1:D:663:GLU:O	1:D:664:TYR:HB2	1.96	0.64
1:A:491:MET:HE1	1:A:514:LEU:CB	2.15	0.64
1:A:426:GLY:HA3	1:A:429:ALA:CB	2.14	0.64
1:A:481:TYR:CD1	1:A:481:TYR:N	2.66	0.63
1:A:187:ARG:NH2	1:A:438:ARG:NH2	2.46	0.63
1:A:348:HIS:HE1	1:A:354:TRP:NE1	1.96	0.63
2:X:17:DG:OP2	2:X:17:DG:H8	1.80	0.63
1:A:398:ILE:HD12	1:A:491:MET:HG2	1.81	0.63
1:A:187:ARG:CZ	1:A:438:ARG:NH2	2.62	0.63
1:D:38:LYS:HB3	1:D:253:VAL:CG1	2.29	0.63
1:A:342:ASP:OD1	1:A:346:ARG:NH1	2.30	0.62
2:X:18:DC:C4	2:X:19:DT:C4	2.87	0.62
1:A:606:GLU:OE1	1:A:609:ARG:NH1	2.32	0.62
1:A:419:GLY:HA2	1:A:425:ILE:CD1	2.30	0.62
2:X:2:DC:N3	3:Y:17:DG:N2	2.44	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TRP:HZ2	1:A:454:GLN:HG2	1.64	0.62
1:D:30:VAL:HB	1:D:253:VAL:HG22	1.82	0.62
1:D:343:TRP:HA	1:D:346:ARG:HG3	1.80	0.61
2:X:19:DT:O4	3:Y:2:DC:N3	2.33	0.61
3:Y:3:DA:OP2	3:Y:3:DA:C8	2.52	0.61
1:D:426:GLY:O	1:D:430:LEU:N	2.29	0.61
1:A:425:ILE:N	1:A:425:ILE:HD13	2.16	0.61
1:D:436:TRP:CE2	1:D:440:HIS:CD2	2.89	0.61
1:A:188:LYS:CE	1:A:198:ASP:OD2	2.47	0.61
1:A:423:ARG:NH2	1:A:467:PHE:CE1	2.68	0.60
1:A:486:PHE:CE2	1:A:535:ILE:HD13	2.36	0.60
1:A:419:GLY:CA	1:A:425:ILE:HG13	2.31	0.60
1:A:487:LEU:HD13	1:A:517:LEU:HD22	1.83	0.60
1:D:427:ASP:OD1	1:D:427:ASP:C	2.38	0.60
3:Y:17:DG:OP2	3:Y:17:DG:C8	2.55	0.60
1:D:365:ALA:HB2	3:Y:20:DT:H3	1.67	0.60
1:A:348:HIS:ND1	1:A:354:TRP:CE2	2.68	0.60
1:A:116:TYR:CE2	1:A:124:ILE:CD1	2.77	0.60
1:D:116:TYR:HE2	1:D:124:ILE:CD1	2.07	0.59
1:A:418:ILE:O	1:A:425:ILE:HD12	2.02	0.59
1:D:238:GLU:OE2	1:D:241:ARG:NH2	2.22	0.59
3:Y:3:DA:H2"	3:Y:4:DG:C8	2.38	0.59
2:X:18:DC:N4	2:X:19:DT:C7	2.66	0.59
1:D:345:THR:O	1:D:346:ARG:C	2.36	0.59
2:X:18:DC:N4	2:X:19:DT:H72	2.17	0.59
1:D:393:ARG:HH22	1:D:420:ARG:NH1	1.99	0.59
2:X:18:DC:C4	2:X:19:DT:C5	2.91	0.59
1:D:332:ASP:HB3	1:D:335:ALA:H	1.67	0.59
1:D:459:ARG:HD2	3:Y:9:DC:C4'	2.32	0.58
1:D:477:ALA:O	1:D:481[B]:TYR:HB3	2.04	0.58
1:A:440:HIS:O	1:A:441:HIS:CG	2.57	0.58
1:D:291:ARG:NH2	4:D:1665:ANP:HNB1	2.02	0.58
1:D:374:LEU:HB3	1:D:379:ILE:HB	1.85	0.58
1:D:491:MET:CE	1:D:514:LEU:CB	2.73	0.58
1:D:389:PHE:O	1:D:395:ILE:HD12	2.04	0.58
1:D:428:THR:HG1	3:Y:10:DG:P	2.28	0.57
1:D:38:LYS:HB3	1:D:253:VAL:HG11	1.87	0.57
1:D:663:GLU:O	1:D:664:TYR:CB	2.52	0.57
2:X:6:DC:H2"	2:X:7:DT:H71	1.86	0.57
2:X:18:DC:C4	2:X:19:DT:C7	2.87	0.57
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:480:ASN:O	1:D:481[A]:TYR:CB	2.49	0.57
2:X:20:DT:H4'	2:X:21:DT:C5'	2.34	0.57
1:A:660:GLN:CG	1:A:661:PRO:HD2	2.35	0.57
1:D:110[B]:ARG:NH1	1:D:110[B]:ARG:CB	2.68	0.57
1:A:487:LEU:CD1	1:A:517:LEU:CD2	2.82	0.57
2:X:5:DC:N4	3:Y:14:DG:H1	2.02	0.57
1:D:206:LEU:HD21	1:D:213:VAL:HG11	1.87	0.56
1:D:528:GLU:HG2	1:D:529:ALA:N	2.19	0.56
1:A:587:GLU:CD	1:A:630:ARG:HH12	2.09	0.56
1:D:459:ARG:NH2	2:X:12:DG:H21	2.03	0.56
1:A:436:TRP:CZ2	1:A:454:GLN:HG2	2.40	0.56
1:D:330:ALA:HB1	1:D:335:ALA:HB3	1.86	0.56
1:A:314:THR:HG21	1:A:316:LYS:HE3	1.88	0.56
3:Y:20:DT:C2'	3:Y:21:DT:OP2	2.53	0.56
1:A:307:ASN:OD1	1:A:605:GLU:HG2	2.06	0.55
1:A:660:GLN:N	1:A:660:GLN:OE1	2.34	0.55
1:D:12:ALA:O	1:D:40:ARG:NH2	2.26	0.55
1:D:408:PRO:HB3	1:D:445:LEU:HD23	1.87	0.55
1:D:571:HIS:CE1	3:Y:22:DT:H1'	2.41	0.55
2:X:14:DA:N1	3:Y:5:DT:O2	2.40	0.55
1:D:23:HIS:O	1:D:24:PHE:HB3	2.07	0.55
1:D:479:ASP:O	1:D:480:ASN:HB2	2.07	0.55
1:A:362:ARG:NH2	2:X:21:DT:O2	2.40	0.54
1:D:307:ASN:OD1	1:D:605:GLU:HG2	2.07	0.54
1:D:393:ARG:NH2	1:D:420:ARG:NH2	2.34	0.54
1:D:491:MET:HE3	1:D:514:LEU:CB	2.35	0.54
1:D:129:MET:CE	1:D:141:PRO:HG3	2.38	0.54
1:A:348:HIS:ND1	1:A:354:TRP:CH2	2.72	0.54
1:D:110[B]:ARG:HH11	1:D:110[B]:ARG:CB	2.20	0.54
1:A:291:ARG:NH2	4:A:1665:ANP:HNB1	2.06	0.54
1:D:423:ARG:N	1:D:425:ILE:CD1	2.66	0.54
2:X:15:DC:N3	3:Y:4:DG:N2	2.51	0.54
2:X:20:DT:H4'	2:X:21:DT:H5"	1.89	0.54
1:D:656:ASP:HB2	1:D:657:PRO:HD2	1.89	0.54
1:A:425:ILE:O	1:A:427:ASP:N	2.41	0.54
1:A:426:GLY:O	1:A:430:LEU:N	2.27	0.54
1:A:129:MET:CE	1:A:141:PRO:HG3	2.38	0.53
1:A:344:LEU:HD12	1:A:374:LEU:HD22	1.91	0.53
1:D:595:GLY:O	1:D:599:GLU:HG3	2.07	0.53
1:A:187:ARG:CZ	1:A:438:ARG:HH22	2.21	0.53
1:A:419:GLY:HA2	1:A:425:ILE:CG1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TRP:HE1	1:A:455:ASN:HB3	1.73	0.53
1:D:436:TRP:CZ2	1:D:440:HIS:HD2	2.26	0.53
1:D:480:ASN:O	1:D:481[B]:TYR:HB3	2.07	0.53
1:A:295:ARG:HG3	1:A:321:ALA:HB1	1.89	0.53
1:A:423:ARG:H	1:A:425:ILE:CD1	2.21	0.53
1:D:395:ILE:O	1:D:399:LEU:HG	2.08	0.53
2:X:18:DC:N3	2:X:19:DT:C4	2.76	0.53
1:D:656:ASP:O	1:D:658:TYR:O	2.27	0.53
1:A:486:PHE:CE2	1:A:535:ILE:CD1	2.91	0.53
1:A:571:HIS:CE1	2:X:22:DT:H1'	2.44	0.53
1:A:336:GLU:OE1	1:A:630:ARG:NH2	2.42	0.53
1:A:179:GLU:OE2	1:A:183:ARG:HD2	2.08	0.53
1:A:545:LEU:HD13	1:A:552:ARG:HG3	1.91	0.53
1:D:377:VAL:HG12	1:D:377:VAL:O	2.09	0.53
1:D:437:ALA:O	1:D:441:HIS:C	2.46	0.53
2:X:15:DC:C5	2:X:16:DT:O4	2.62	0.53
1:A:393:ARG:NH2	1:A:420:ARG:NH1	2.57	0.52
1:A:633:PHE:HB3	2:X:20:DT:H72	1.89	0.52
1:D:257:ASP:O	1:D:609:ARG:HG2	2.08	0.52
1:D:140:GLN:OE1	1:D:142:ARG:NH2	2.42	0.52
1:D:528:GLU:HG2	1:D:529:ALA:H	1.74	0.52
1:A:120:ASP:OD1	1:A:403:ARG:NH2	2.43	0.52
1:A:129:MET:HA	1:A:132:ILE:HD12	1.90	0.52
1:A:374:LEU:HB3	1:A:379:ILE:HB	1.92	0.52
3:Y:9:DC:H2"	3:Y:10:DG:C8	2.45	0.52
1:D:428:THR:OG1	3:Y:10:DG:P	2.68	0.52
1:A:138:GLU:CG	1:A:139:THR:N	2.62	0.52
1:A:384:VAL:HB	1:A:568:MET:HB3	1.91	0.52
1:D:246:ARG:CD	1:D:247:ASP:OD1	2.58	0.52
1:A:456:ILE:HG12	1:A:458:ASP:OD1	2.10	0.51
1:A:595:GLY:O	1:A:599:GLU:HG3	2.11	0.51
1:A:246:ARG:HD2	1:A:247:ASP:OD1	2.10	0.51
3:Y:2:DC:H2"	3:Y:3:DA:OP2	2.10	0.51
1:D:327:PHE:HA	1:D:624:MET:O	2.10	0.51
1:A:45:ARG:NH1	1:A:225:HIS:NE2	2.59	0.51
1:A:401:TYR:OH	1:A:420:ARG:O	2.27	0.51
1:A:654:THR:CG2	1:A:662:ILE:O	2.58	0.51
1:D:32:ALA:CB	1:D:286:LEU:HB2	2.41	0.51
1:D:37:GLY:HA2	4:D:1665:ANP:O1A	2.11	0.51
1:A:257:ASP:O	1:A:609:ARG:HG2	2.11	0.51
1:A:403:ARG:NH1	1:A:410:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:ILE:HG23	1:A:456:ILE:O	2.11	0.51
1:D:426:GLY:O	1:D:430:LEU:CB	2.54	0.51
1:D:348:HIS:CE1	1:D:354:TRP:CE2	2.99	0.51
1:A:42:LEU:CD1	1:A:253:VAL:HG21	2.40	0.51
1:D:187:ARG:NH2	1:D:415:ARG:HH22	2.09	0.51
1:D:23:HIS:CE1	1:D:28:ALA:HB2	2.46	0.50
1:D:188:LYS:CE	1:D:198:ASP:OD2	2.59	0.50
1:D:432:LYS:HE3	1:D:457:LEU:HD22	1.92	0.50
1:A:352[A]:ARG:NH2	1:A:620:GLU:HG3	2.26	0.50
1:D:441:HIS:O	1:D:443:SER:N	2.44	0.50
1:A:478:ALA:HB2	1:A:486:PHE:CE1	2.46	0.50
1:A:632:GLN:O	2:X:20:DT:C7	2.60	0.50
1:D:295:ARG:HD2	1:D:324:PRO:HA	1.94	0.50
1:D:389:PHE:O	1:D:395:ILE:CD1	2.60	0.50
1:D:650:GLY:C	1:D:651:LEU:HD12	2.31	0.50
1:A:477:ALA:HA	1:A:481:TYR:HE2	1.74	0.50
1:D:248:ARG:HH22	1:D:280:ASP:CG	2.14	0.50
1:D:437:ALA:O	1:D:441:HIS:O	2.30	0.50
2:X:12:DG:H2"	2:X:13:DC:C6	2.47	0.50
1:D:375[A]:ARG:HG3	1:D:375[A]:ARG:HH11	1.76	0.50
1:D:384:VAL:HB	1:D:568:MET:HB3	1.93	0.50
1:A:7:PRO:CB	1:A:80:LEU:HD22	2.40	0.50
1:A:140:GLN:OE1	1:A:142:ARG:NH2	2.45	0.50
1:A:333:HIS:O	1:A:336:GLU:HB3	2.12	0.50
1:A:394:GLU:HG2	1:A:510:ARG:HB3	1.92	0.50
1:A:654:THR:HG22	1:A:662:ILE:O	2.10	0.50
3:Y:17:DG:C5	3:Y:18:DT:C4	2.99	0.50
1:A:621:ARG:HA	9:A:2055:HOH:O	2.12	0.49
1:D:7:PRO:CB	1:D:80:LEU:HD22	2.39	0.49
1:D:440:HIS:N	1:D:440:HIS:HD1	2.10	0.49
1:D:632:GLN:HG3	1:D:633:PHE:N	2.25	0.49
1:A:436:TRP:NE1	1:A:455:ASN:HB3	2.27	0.49
1:A:587:GLU:CD	1:A:630:ARG:NH1	2.65	0.49
1:A:377:VAL:O	1:A:377:VAL:CG1	2.60	0.49
1:A:486:PHE:CD2	1:A:535:ILE:CD1	2.96	0.49
1:D:274:PHE:HA	9:D:2055:HOH:O	2.11	0.49
3:Y:20:DT:H1'	3:Y:21:DT:O5'	2.12	0.49
1:A:246:ARG:CD	1:A:247:ASP:OD1	2.61	0.49
3:Y:3:DA:OP2	3:Y:3:DA:H2'	2.12	0.49
1:A:362:ARG:HG2	1:A:590:LEU:O	2.13	0.49
1:D:436:TRP:CE2	1:D:440:HIS:NE2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:15:DC:C4	2:X:16:DT:C4	3.01	0.49
2:X:18:DC:C1'	2:X:19:DT:H5"	2.31	0.49
1:D:354:TRP:CH2	1:D:379:ILE:HG23	2.47	0.49
2:X:18:DC:H2"	2:X:19:DT:C5'	2.43	0.49
3:Y:9:DC:H2"	3:Y:10:DG:H8	1.78	0.49
1:D:382:ARG:HA	1:D:557:ASN:OD1	2.13	0.48
1:D:263:PHE:CD1	1:D:263:PHE:C	2.87	0.48
2:X:14:DA:H61	3:Y:5:DT:H3	0.65	0.48
1:D:472:GLU:OE1	1:D:472:GLU:HA	2.12	0.48
1:D:508:GLN:HA	1:D:511:LEU:HG	1.95	0.48
1:D:621:ARG:HA	9:D:2063:HOH:O	2.13	0.48
1:A:333:HIS:HD2	1:A:369:VAL:HG21	1.78	0.48
1:A:336:GLU:OE2	1:A:625:THR:OG1	2.23	0.48
1:D:333:HIS:O	1:D:336:GLU:HB3	2.13	0.48
1:A:110[B]:ARG:HH11	1:A:110[B]:ARG:HB2	1.77	0.48
1:D:382:ARG:NH2	9:D:2073:HOH:O	2.41	0.48
1:A:393:ARG:HH21	1:A:420:ARG:CZ	2.26	0.48
1:D:29:LEU:HB2	1:D:274:PHE:CD2	2.48	0.48
1:D:336:GLU:OE1	1:D:630:ARG:NH2	2.45	0.47
2:X:20:DT:H5'	2:X:20:DT:O2	2.13	0.47
1:A:129:MET:HE2	1:A:141:PRO:HG3	1.95	0.47
1:A:73:MET:HB3	1:A:73:MET:HE2	1.72	0.47
1:A:423:ARG:NH2	1:A:467:PHE:CD1	2.82	0.47
3:Y:3:DA:H1'	3:Y:4:DG:C8	2.50	0.47
1:D:428:THR:OG1	3:Y:10:DG:OP1	2.32	0.47
1:D:23:HIS:O	1:D:24:PHE:CB	2.58	0.47
1:D:348:HIS:ND1	1:D:354:TRP:CE2	2.82	0.47
1:A:443:SER:HB2	1:A:446:THR:HG23	1.97	0.47
1:A:457:LEU:HD13	1:A:457:LEU:O	2.14	0.47
1:A:632:GLN:HG2	1:A:633:PHE:CD2	2.50	0.47
1:D:246:ARG:HD2	1:D:247:ASP:OD1	2.15	0.47
1:D:587:GLU:CD	1:D:630:ARG:HH12	2.18	0.47
1:D:656:ASP:HB2	1:D:657:PRO:CD	2.44	0.47
2:X:4:DA:C1'	2:X:5:DC:OP2	2.45	0.47
1:A:248:ARG:HH22	1:A:280:ASP:CG	2.17	0.47
1:A:395:ILE:O	1:A:399:LEU:HG	2.15	0.47
1:A:127:GLU:HG2	1:A:187:ARG:NH2	2.29	0.47
1:A:579:PRO:HA	1:A:619:MET:HB2	1.97	0.47
1:D:129:MET:HE2	1:D:141:PRO:HG3	1.97	0.47
1:D:179:GLU:OE2	1:D:183:ARG:HD2	2.15	0.46
1:A:429:ALA:O	1:A:433:LEU:N	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:ASP:OD2	1:D:310:ARG:NH1	2.48	0.46
2:X:6:DC:H2"	2:X:7:DT:C7	2.45	0.46
1:A:330:ALA:HB1	1:A:335:ALA:HB3	1.97	0.46
1:D:409:ALA:CB	9:D:2080:HOH:O	2.58	0.46
1:A:116:TYR:HE2	1:A:124:ILE:CD1	2.19	0.46
1:D:348:HIS:CE1	1:D:354:TRP:CZ2	3.03	0.46
3:Y:17:DG:C6	3:Y:18:DT:C4	3.04	0.46
1:D:588:GLN:NE2	1:D:597:ILE:HD11	2.31	0.46
1:A:480:ASN:C	1:A:481:TYR:CD1	2.89	0.46
1:D:352[B]:ARG:NH1	1:D:356:GLU:OE1	2.49	0.46
1:D:432:LYS:CB	1:D:457:LEU:HD22	2.44	0.46
2:X:18:DC:H1'	2:X:19:DT:C5'	2.33	0.46
2:X:1:DA:H3'	2:X:2:DC:C6	2.50	0.46
2:X:3:DG:H2"	2:X:4:DA:H8	1.78	0.46
1:D:336:GLU:OE2	1:D:625:THR:OG1	2.29	0.45
1:D:632:GLN:O	1:D:634:GLY:N	2.49	0.45
2:X:1:DA:P	2:X:2:DC:OP1	2.73	0.45
1:A:436:TRP:CD1	1:A:455:ASN:HB3	2.51	0.45
1:A:508:GLN:HA	1:A:511:LEU:HG	1.98	0.45
1:D:264:ARG:O	1:D:264:ARG:HG2	2.17	0.45
1:D:487:LEU:HD13	1:D:517:LEU:HD22	1.93	0.45
3:Y:20:DT:C1'	3:Y:21:DT:H5"	2.16	0.45
1:A:654:THR:O	1:A:661:PRO:HA	2.17	0.45
1:D:418:ILE:HG23	1:D:425:ILE:HG23	1.98	0.45
1:D:362:ARG:NH2	3:Y:21:DT:O2	2.50	0.45
2:X:5:DC:OP2	2:X:5:DC:O4'	2.34	0.45
1:D:24:PHE:CE2	1:D:25:THR:HG23	2.51	0.45
1:D:436:TRP:CZ3	1:D:447:ALA:HA	2.52	0.45
1:A:88:TRP:CD2	1:A:98:ARG:NH2	2.84	0.45
1:D:110[B]:ARG:NH1	1:D:110[B]:ARG:HB3	2.31	0.45
1:D:342:ASP:OD2	1:D:346:ARG:CZ	2.65	0.44
1:D:517:LEU:HD23	1:D:517:LEU:O	2.17	0.44
1:D:362:ARG:HG2	1:D:590:LEU:O	2.16	0.44
1:A:491:MET:HE1	1:A:514:LEU:HD13	2.00	0.44
1:D:517:LEU:HD23	1:D:517:LEU:C	2.38	0.44
1:D:24:PHE:O	1:D:45:ARG:NH2	2.50	0.44
1:D:323:GLN:CD	1:D:621:ARG:HD2	2.37	0.44
3:Y:5:DT:H2"	3:Y:6:DG:C8	2.52	0.44
1:A:6:GLY:HA3	9:A:2001:HOH:O	2.16	0.44
1:A:110[B]:ARG:NH1	1:A:110[B]:ARG:CB	2.80	0.44
1:D:62:ALA:HA	1:D:225:HIS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:LYS:HB3	1:D:457:LEU:CD2	2.46	0.44
1:A:327:PHE:HA	1:A:624:MET:O	2.18	0.44
1:D:248:ARG:NH2	1:D:280:ASP:OD2	2.51	0.44
1:D:361:TYR:O	1:D:569:THR:HA	2.17	0.44
1:D:157:THR:O	1:D:160:ASP:HB2	2.18	0.44
1:D:495:GLY:O	1:D:498:ASP:OD1	2.36	0.44
1:D:587:GLU:CD	1:D:630:ARG:NH1	2.70	0.44
1:A:323:GLN:CD	1:A:621:ARG:HD2	2.39	0.43
1:A:662:ILE:O	1:A:662:ILE:CG2	2.64	0.43
1:A:395:ILE:HG23	1:A:517:LEU:HD12	1.99	0.43
1:A:423:ARG:N	1:A:425:ILE:HD11	2.33	0.43
1:A:483:PRO:O	1:A:487:LEU:HG	2.17	0.43
1:D:129:MET:HA	1:D:132:ILE:HD12	1.99	0.43
1:D:393:ARG:CZ	1:D:420:ARG:HH12	2.28	0.43
1:D:528:GLU:O	1:D:531:VAL:HG23	2.19	0.43
2:X:18:DC:C5	2:X:19:DT:C7	2.96	0.43
1:A:528:GLU:HG2	1:A:529:ALA:N	2.33	0.43
1:D:27:PRO:HA	1:D:250:LEU:O	2.18	0.43
1:D:478:ALA:C	1:D:480:ASN:H	2.21	0.43
1:A:528:GLU:O	1:A:531:VAL:HG23	2.19	0.43
1:D:120:ASP:OD1	1:D:403:ARG:NH2	2.51	0.43
1:D:418:ILE:CG2	1:D:419:GLY:N	2.82	0.43
1:A:344:LEU:HD11	1:A:359:ILE:HD11	2.01	0.43
1:D:347:LEU:HD22	1:D:352[A]:ARG:NH2	2.33	0.43
1:A:21:ALA:HA	1:A:45:ARG:HB2	2.00	0.43
1:D:42:LEU:HD12	1:D:42:LEU:HA	1.83	0.43
1:D:333:HIS:HD2	1:D:369:VAL:HG21	1.84	0.43
1:A:402:ALA:O	1:A:406:LEU:HD23	2.19	0.43
1:A:498:ASP:HB3	1:A:501:ARG:HH21	1.83	0.43
1:A:500:LEU:O	1:A:504:GLY:CA	2.67	0.43
1:D:293:SER:OG	1:D:296:VAL:HG13	2.19	0.43
1:D:329:ARG:HH22	1:D:664:TYR:HB3	1.84	0.43
2:X:3:DG:C6	3:Y:16:DC:N3	2.86	0.43
1:A:505:GLN:H	1:A:507:GLY:H	1.67	0.42
2:X:20:DT:C4'	2:X:21:DT:H5"	2.48	0.42
1:A:207:PHE:CG	1:A:214:LEU:HD13	2.54	0.42
1:A:344:LEU:HD23	1:A:344:LEU:HA	1.86	0.42
1:A:573:ALA:O	1:A:574:LYS:C	2.58	0.42
1:D:14:ASN:HB2	1:D:15:PRO:HD2	2.00	0.42
1:D:482:GLU:HA	1:D:483:PRO:HD3	1.82	0.42
3:Y:19:DT:H3'	3:Y:20:DT:H2'	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PHE:HB2	1:D:228:GLU:HG3	2.00	0.42
1:D:418:ILE:HG23	1:D:419:GLY:N	2.34	0.42
1:A:401:TYR:CE1	1:A:417:ILE:HD13	2.54	0.42
1:A:633:PHE:O	1:A:633:PHE:CD1	2.72	0.42
2:X:19:DT:C4	3:Y:2:DC:N3	2.87	0.42
1:A:323:GLN:HA	1:A:324:PRO:HD3	1.92	0.42
1:D:308:THR:HG23	1:D:309:GLU:HG2	2.02	0.42
1:D:581:VAL:HB	1:D:618:ALA:HB2	2.02	0.42
1:A:238:GLU:OE2	1:A:241:ARG:NH2	2.29	0.42
1:D:32:ALA:HB1	1:D:286:LEU:HB2	2.01	0.42
1:D:73:MET:HB3	1:D:73:MET:HE2	1.66	0.42
1:D:256:PRO:HD2	1:D:313:LYS:NZ	2.35	0.42
1:D:286:LEU:N	1:D:286:LEU:CD1	2.82	0.42
1:D:352[B]:ARG:HA	1:D:352[B]:ARG:HD3	1.91	0.42
2:X:1:DA:P	9:X:2001:HOH:O	2.77	0.42
1:A:397:ASP:OD2	1:A:496:TYR:OH	2.29	0.42
1:A:632:GLN:O	2:X:20:DT:H72	2.20	0.42
1:D:591:LEU:HD12	1:D:591:LEU:HA	1.92	0.42
1:D:363:THR:OG1	1:D:366:GLN:OE1	2.22	0.42
1:A:487:LEU:CD1	1:A:517:LEU:HD21	2.44	0.42
1:D:74:ARG:NH1	9:D:2016:HOH:O	2.53	0.42
1:D:246:ARG:HD3	1:D:247:ASP:OD1	2.19	0.42
1:D:500:LEU:O	1:D:504:GLY:CA	2.68	0.42
1:D:660:GLN:HA	1:D:661:PRO:HD2	1.72	0.42
1:A:23:HIS:CE1	1:A:282:LYS:HD3	2.55	0.41
1:D:23:HIS:CE1	1:D:282:LYS:HD3	2.54	0.41
1:D:172:LEU:HD23	1:D:172:LEU:HA	1.89	0.41
1:D:505:GLN:H	1:D:507:GLY:H	1.66	0.41
1:D:588:GLN:HE22	1:D:597:ILE:HD11	1.85	0.41
1:A:64:THR:OG1	1:A:70:ALA:HB2	2.19	0.41
1:D:74:ARG:HH11	1:D:74:ARG:HD2	1.72	0.41
1:D:259:SER:O	1:D:609:ARG:HD2	2.21	0.41
1:D:344:LEU:HD23	1:D:344:LEU:HA	1.85	0.41
1:A:179:GLU:OE1	1:A:179:GLU:HA	2.20	0.41
1:D:291:ARG:NH2	4:D:1665:ANP:N3B	2.67	0.41
1:A:150[A]:ARG:HB2	1:A:150[A]:ARG:NH1	2.36	0.41
1:A:264:ARG:HG2	1:A:264:ARG:O	2.21	0.41
1:A:491:MET:CE	1:A:514:LEU:HD13	2.50	0.41
1:D:379:ILE:O	9:D:2072:HOH:O	2.22	0.41
2:X:2:DC:N4	3:Y:16:DC:N4	2.69	0.41
1:A:63:VAL:HA	1:A:90:SER:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:LEU:HD23	1:D:399:LEU:HA	1.85	0.41
1:A:408:PRO:HB3	1:A:445:LEU:HD23	2.02	0.41
1:A:423:ARG:N	1:A:425:ILE:CD1	2.84	0.41
1:D:159:ASP:O	1:D:162:ASP:HB2	2.21	0.41
1:D:196:PHE:O	1:D:199:LEU:HB2	2.21	0.41
1:A:154:ASN:O	1:A:234[B]:ARG:NH1	2.43	0.41
1:A:157:THR:O	1:A:160:ASP:HB2	2.21	0.41
1:A:187:ARG:HG3	1:A:187:ARG:HH11	1.85	0.41
1:A:293:SER:OG	1:A:296:VAL:HG13	2.20	0.41
1:A:586:VAL:HG12	1:A:642:SER:HB3	2.03	0.41
1:D:64:THR:OG1	1:D:70:ALA:HB2	2.21	0.41
1:D:292:SER:OG	1:D:618:ALA:O	2.31	0.41
1:D:308:THR:O	1:D:309:GLU:HB2	2.21	0.41
1:D:377:VAL:O	1:D:377:VAL:CG1	2.69	0.41
1:A:202:GLU:OE1	1:A:205:ARG:HD3	2.20	0.41
1:A:303:LEU:HB2	1:A:648:ILE:CG2	2.51	0.41
1:A:480:ASN:C	1:A:481:TYR:CG	2.94	0.41
1:D:663:GLU:C	1:D:664:TYR:HD1	2.22	0.41
2:X:1:DA:H3'	2:X:2:DC:C5	2.56	0.41
2:X:8:DG:H1	3:Y:11:DC:H42	1.67	0.41
1:D:624:MET:H	1:D:624:MET:HG2	1.69	0.40
1:A:23:HIS:O	1:A:24:PHE:CB	2.68	0.40
3:Y:20:DT:OP1	3:Y:20:DT:C6	2.74	0.40
1:D:187:ARG:CZ	1:D:438:ARG:HH22	2.35	0.40
1:D:140:GLN:OE1	1:D:142:ARG:CZ	2.69	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
1	A	661/665 (99%)	609 (92%)	41 (6%)	11 (2%)	9 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	661/665 (99%)	619 (94%)	29 (4%)	13 (2%)	7 8
All	All	1322/1330 (99%)	1228 (93%)	70 (5%)	24 (2%)	8 10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	421	PRO
1	D	441	HIS
1	D	442	THR
1	D	480	ASN
1	D	481[A]	TYR
1	D	481[B]	TYR
1	A	423	ARG
1	A	426	GLY
1	A	441	HIS
1	A	442	THR
1	D	633	PHE
1	D	24	PHE
1	D	482	GLU
1	A	24	PHE
1	A	133	PRO
1	A	460	GLY
1	D	133	PRO
1	A	592	PRO
1	D	423	ARG
1	D	586	VAL
1	D	592	PRO
1	A	504	GLY
1	D	661	PRO
1	A	456	ILE

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	538/536 (100%)	522 (97%)	16 (3%)	41 55
1	D	538/536 (100%)	512 (95%)	26 (5%)	25 34
All	All	1076/1072 (100%)	1034 (96%)	42 (4%)	32 44

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	42	LEU
1	A	127	GLU
1	A	139	THR
1	A	325	VAL
1	A	345	THR
1	A	346	ARG
1	A	394	GLU
1	A	434	MET
1	A	480	ASN
1	A	481	TYR
1	A	528	GLU
1	A	592	PRO
1	A	624	MET
1	A	663	GLU
1	A	664	TYR
1	D	11	GLN
1	D	42	LEU
1	D	45	ARG
1	D	110[A]	ARG
1	D	110[B]	ARG
1	D	127	GLU
1	D	205	ARG
1	D	286	LEU
1	D	296	VAL
1	D	345	THR
1	D	394	GLU
1	D	417	ILE
1	D	418	ILE
1	D	420	ARG
1	D	425	ILE
1	D	427	ASP
1	D	433	LEU
1	D	438	ARG
1	D	439	THR

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Mol	Chain	Res	Type
1	D	440	HIS
1	D	528	GLU
1	D	602	SER
1	D	624	MET
1	D	633	PHE
1	D	655	VAL
1	D	663	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	ASN
1	A	121	GLN
1	A	236	GLN
1	A	270	ASN
1	A	480	ASN
1	D	67	ASN
1	D	236	GLN
1	D	301	ASN
1	D	364	ASN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
6	NO3	D	1669	-	1,3,3	3.31	1 (100%)	0,3,3	-	-
6	NO3	A	1669	-	1,3,3	3.82	1 (100%)	0,3,3	-	-
7	GOL	D	1668	-	5,5,5	0.63	0	5,5,5	0.88	0
6	NO3	A	1667	-	1,3,3	3.76	1 (100%)	0,3,3	-	-
6	NO3	D	1667	-	1,3,3	3.79	1 (100%)	0,3,3	-	-
7	GOL	A	1668	-	5,5,5	0.48	0	5,5,5	0.55	0
4	ANP	D	1665	5	29,33,33	3.03	14 (48%)	31,52,52	3.12	11 (35%)
4	ANP	A	1665	5	29,33,33	2.88	12 (41%)	31,52,52	2.80	11 (35%)

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
7	GOL	D	1668	-	-	2/4/4/4	-
7	GOL	A	1668	-	-	4/4/4/4	-
4	ANP	D	1665	5	-	3/14/38/38	0/3/3/3
4	ANP	A	1665	5	-	3/14/38/38	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1665	ANP	PG-O1G	8.46	1.59	1.46
4	D	1665	ANP	PB-O1B	7.33	1.57	1.46
4	A	1665	ANP	PG-O1G	7.20	1.57	1.46
4	A	1665	ANP	PB-O1B	6.33	1.56	1.46
4	A	1665	ANP	PB-O3A	5.69	1.66	1.59
4	D	1665	ANP	PB-O3A	5.35	1.65	1.59
4	D	1665	ANP	PB-N3B	4.24	1.74	1.63
4	D	1665	ANP	PG-N3B	4.23	1.74	1.63
4	A	1665	ANP	C2-N3	4.19	1.38	1.32
6	A	1669	NO3	O1-N	3.82	1.41	1.24
6	D	1667	NO3	O1-N	3.79	1.41	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1665	ANP	PB-N3B	3.76	1.73	1.63
6	A	1667	NO3	O1-N	3.76	1.41	1.24
4	D	1665	ANP	C8-N7	3.72	1.41	1.34
4	A	1665	ANP	PG-N3B	3.70	1.73	1.63
4	A	1665	ANP	C8-N7	3.63	1.41	1.34
4	D	1665	ANP	C2-N3	3.53	1.37	1.32
6	D	1669	NO3	O1-N	3.31	1.39	1.24
4	D	1665	ANP	PA-O1A	3.17	1.62	1.50
4	A	1665	ANP	C5-C4	3.16	1.49	1.40
4	D	1665	ANP	C5-C4	2.85	1.48	1.40
4	A	1665	ANP	C2-N1	2.76	1.39	1.33
4	A	1665	ANP	PA-O1A	2.69	1.60	1.50
4	D	1665	ANP	C4-N3	2.53	1.39	1.35
4	A	1665	ANP	C2'-C1'	-2.33	1.50	1.53
4	D	1665	ANP	O4'-C1'	2.29	1.44	1.41
4	D	1665	ANP	C2-N1	2.16	1.37	1.33
4	D	1665	ANP	C6-N6	2.07	1.41	1.34
4	D	1665	ANP	C2'-C1'	-2.04	1.50	1.53
4	A	1665	ANP	C6-N6	2.03	1.41	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1665	ANP	O1B-PB-N3B	9.38	125.58	111.77
4	A	1665	ANP	O1B-PB-N3B	7.96	123.49	111.77
4	D	1665	ANP	O1G-PG-N3B	-7.30	101.02	111.77
4	D	1665	ANP	O3A-PB-N3B	-7.12	86.85	106.59
4	A	1665	ANP	O3A-PB-N3B	-6.68	88.05	106.59
4	A	1665	ANP	O1G-PG-N3B	-5.17	104.16	111.77
4	A	1665	ANP	PB-O3A-PA	-4.94	115.22	132.62
4	D	1665	ANP	PB-O3A-PA	-4.92	115.29	132.62
4	D	1665	ANP	O5'-PA-O1A	-4.07	93.15	109.07
4	D	1665	ANP	O2G-PG-O3G	3.99	118.27	107.64
4	A	1665	ANP	O2G-PG-O3G	3.61	117.25	107.64
4	A	1665	ANP	C1'-N9-C4	-3.41	120.64	126.64
4	A	1665	ANP	O5'-PA-O1A	-3.16	96.73	109.07
4	A	1665	ANP	O2G-PG-O1G	-2.94	106.06	113.45
4	A	1665	ANP	O2B-PB-O1B	2.92	116.04	109.92
4	D	1665	ANP	C1'-N9-C4	-2.81	121.70	126.64
4	D	1665	ANP	O2A-PA-O1A	2.76	125.88	112.24
4	D	1665	ANP	N6-C6-N1	2.63	124.04	118.57
4	A	1665	ANP	O2B-PB-O3A	-2.25	97.13	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1665	ANP	N3-C2-N1	-2.14	125.33	128.68
4	A	1665	ANP	N6-C6-N1	2.07	122.86	118.57
4	D	1665	ANP	O2G-PG-O1G	-2.04	108.32	113.45

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1665	ANP	PB-N3B-PG-O1G
4	A	1665	ANP	PG-N3B-PB-O1B
4	A	1665	ANP	PG-N3B-PB-O3A
4	D	1665	ANP	PB-N3B-PG-O1G
4	D	1665	ANP	PG-N3B-PB-O1B
4	D	1665	ANP	PG-N3B-PB-O3A
7	D	1668	GOL	C1-C2-C3-O3
7	A	1668	GOL	O1-C1-C2-C3
7	A	1668	GOL	C1-C2-C3-O3
7	A	1668	GOL	O1-C1-C2-O2
7	D	1668	GOL	O2-C2-C3-O3
7	A	1668	GOL	O2-C2-C3-O3

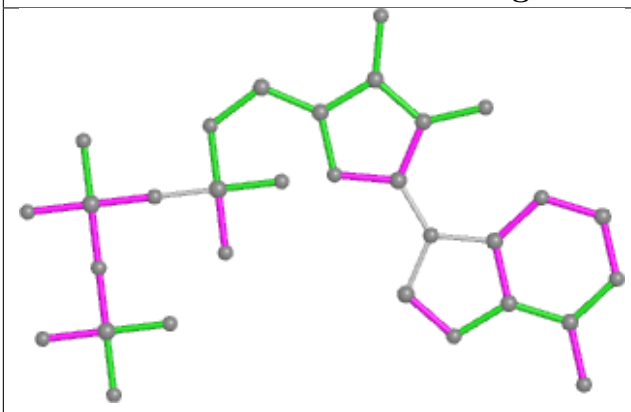
There are no ring outliers.

4 monomers are involved in 6 short contacts:

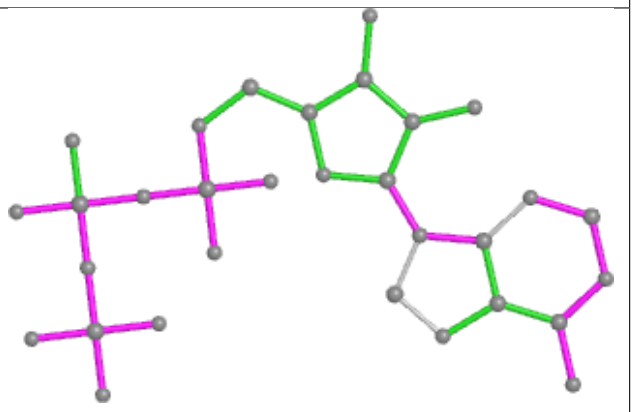
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	1668	GOL	1	0
7	A	1668	GOL	1	0
4	D	1665	ANP	3	0
4	A	1665	ANP	1	0

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

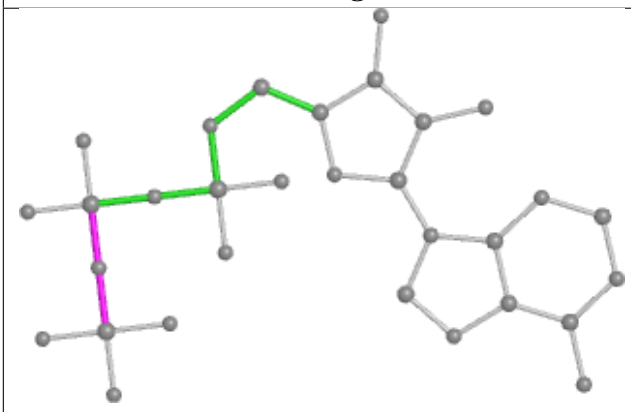
Ligand ANP D 1665



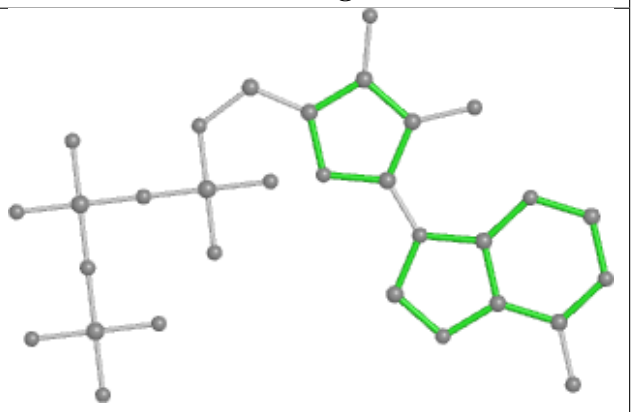
Bond lengths



Bond angles

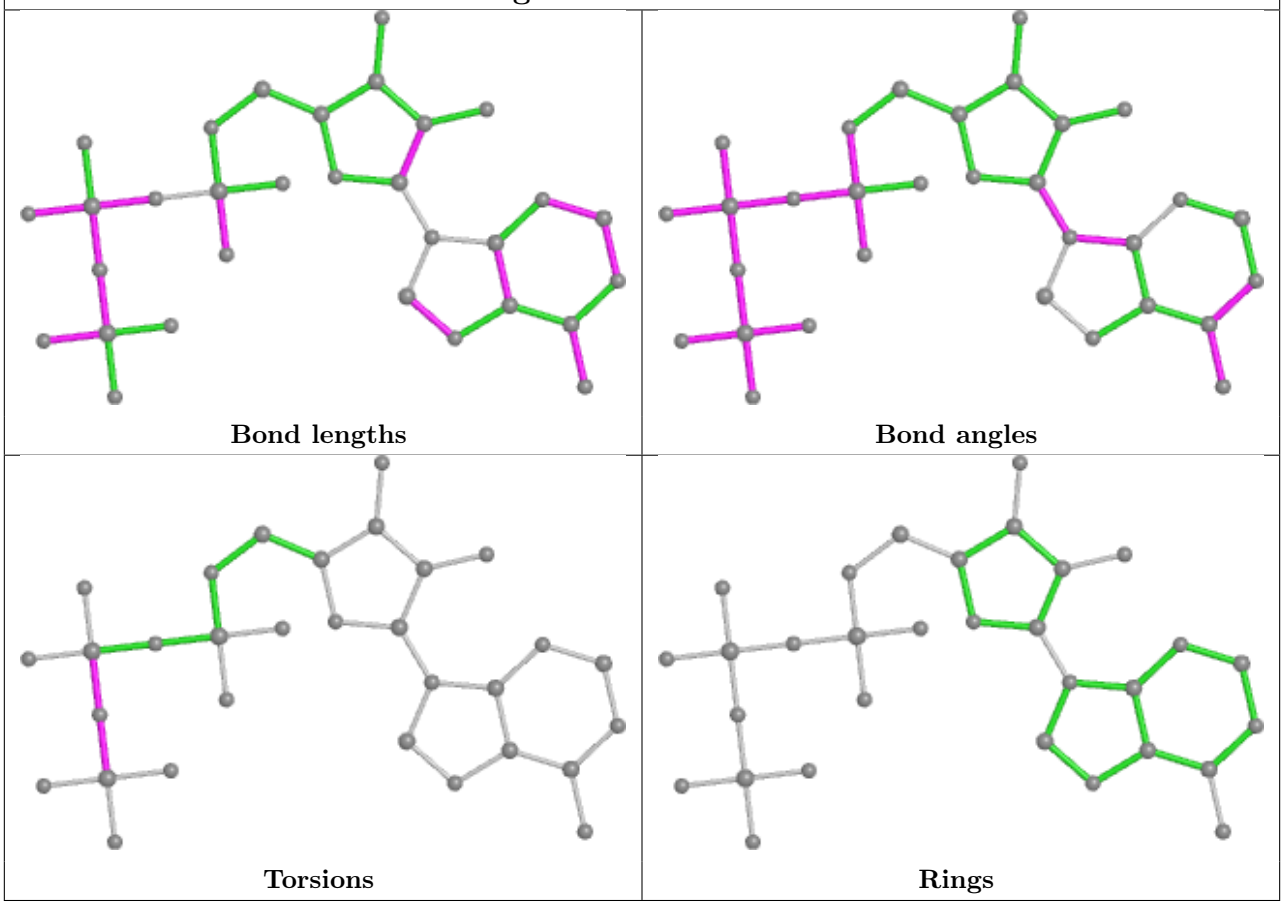


Torsions



Rings

Ligand ANP A 1665



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	A	658/665 (98%)	-0.02	17 (2%)	56	62	26, 56, 116, 155	0
1	D	658/665 (98%)	-0.00	17 (2%)	56	62	26, 56, 118, 184	0
2	X	24/25 (96%)	0.17	1 (4%)	36	42	50, 169, 221, 265	1 (4%)
3	Y	23/25 (92%)	0.55	1 (4%)	35	42	48, 171, 244, 252	1 (4%)
All	All	1363/1380 (98%)	0.00	36 (2%)	56	62	26, 57, 128, 265	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	449	ALA	5.0
3	Y	20	DT	4.8
1	D	452	ALA	4.6
1	D	425	ILE	4.2
1	D	481[A]	TYR	4.1
1	A	4	SER	4.0
1	D	6	GLY	4.0
1	D	436	TRP	3.9
1	A	502	GLN	3.7
1	D	449	ALA	3.5
1	D	662	ILE	3.4
1	A	559	GLY	3.3
1	A	6	GLY	3.2
1	D	502	GLN	3.1
1	A	451	ALA	3.1
1	A	470	LEU	3.0
1	A	452	ALA	2.8
1	D	5	ALA	2.7
1	D	442	THR	2.7
1	D	451	ALA	2.6
1	D	467	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	479	ASP	2.6
2	X	20	DT	2.6
1	A	436	TRP	2.6
1	A	473	ALA	2.5
1	D	455	ASN	2.5
1	A	662	ILE	2.4
1	D	453	GLU	2.4
1	A	408	PRO	2.4
1	A	425	ILE	2.3
1	A	445	LEU	2.2
1	A	442	THR	2.2
1	A	457	LEU	2.1
1	A	664	TYR	2.1
1	D	456	ILE	2.1
1	D	497	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
7	GOL	D	1668	6/6	0.87	0.14	52,57,61,62	0
8	NA	D	1670	1/1	0.87	0.28	45,45,45,45	0
7	GOL	A	1668	6/6	0.90	0.10	56,64,66,70	0
5	MG	A	1666	1/1	0.91	0.05	21,21,21,21	0
6	NO3	D	1669	4/4	0.93	0.44	48,51,51,55	0
6	NO3	A	1667	4/4	0.95	0.09	53,54,59,68	0
8	NA	A	1670	1/1	0.95	0.43	50,50,50,50	0
6	NO3	D	1667	4/4	0.95	0.10	44,50,50,51	0

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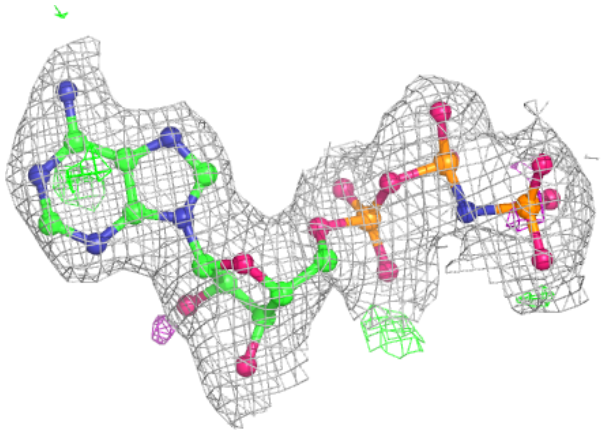
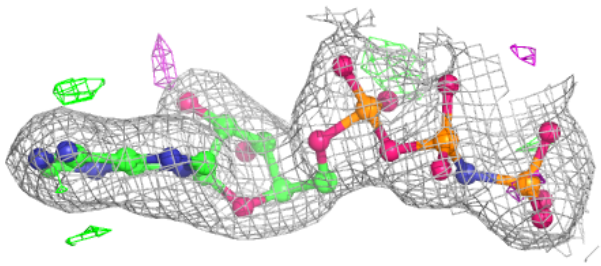
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NO3	A	1669	4/4	0.96	0.14	49,51,52,54	0
5	MG	D	1666	1/1	0.97	0.05	18,18,18,18	0
4	ANP	A	1665	31/31	0.98	0.10	21,29,36,47	0
4	ANP	D	1665	31/31	0.98	0.10	20,28,35,40	0

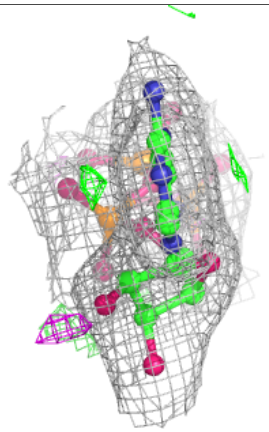
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ANP A 1665:

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

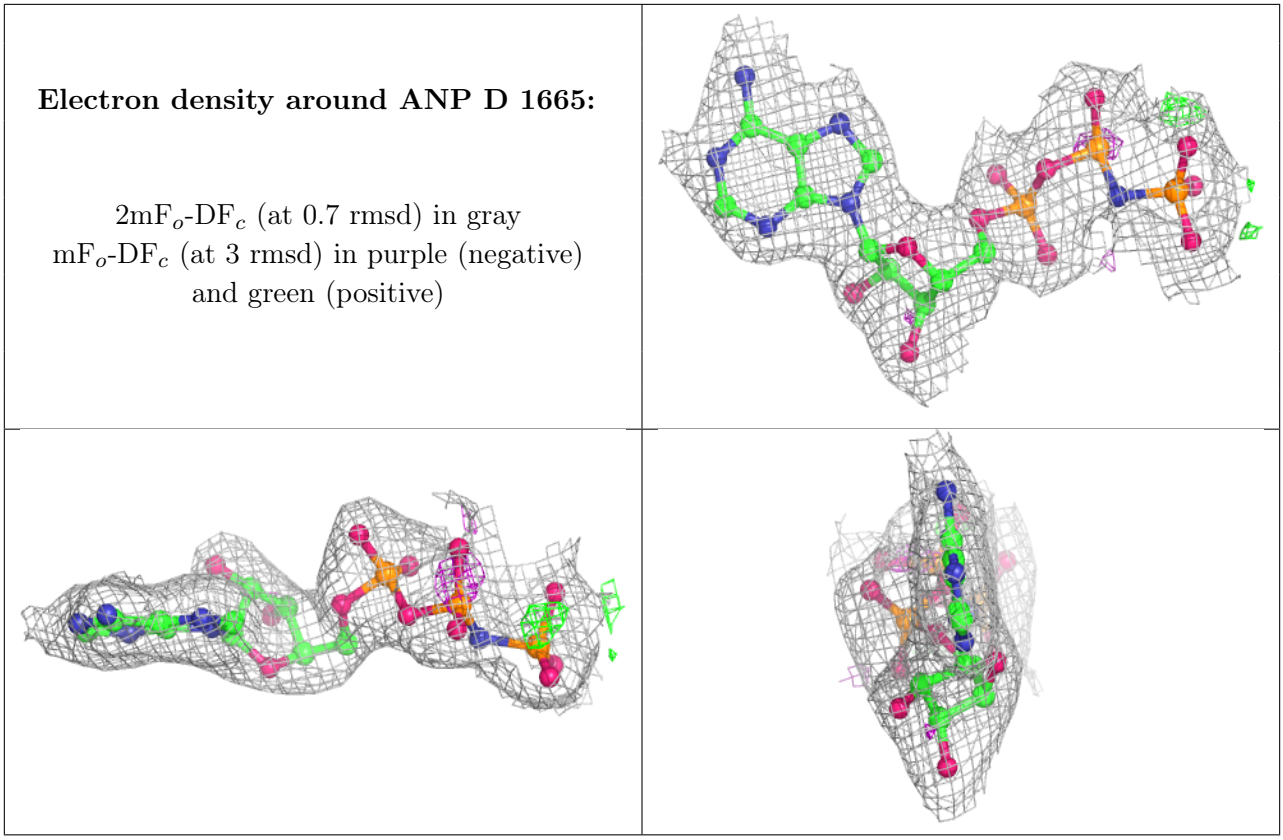






Electron density around ANP D 1665:

$2mF_o$-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.