Full wwPDB X-ray Structure Validation Report (i)

Aug 28, 2023 – 03:39 PM EDT

PDB ID	:	3KK2
Title	:	HIV-1 reverse transcriptase-DNA complex with dATP bound in the nucleotide binding site
Authors	:	Lansdon, E.B.
Deposited on	:	2009-11-04
Resolution	:	2.90 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:

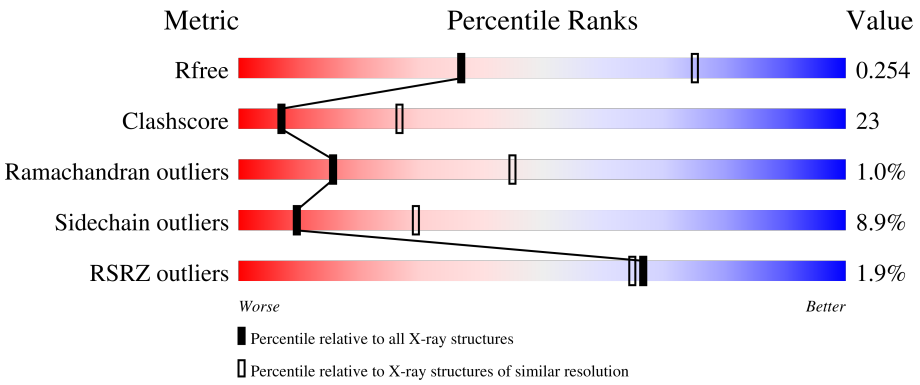
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	560	59% 33% 6% ••
2	B	452	4% 49% 39% • 8%
3	P	21	10% 71% 5% 14%
4	T	27	4% 7% 81% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 8915 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 Reverse transcriptase p66 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4514	2917	753	836	8	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	258	CYS	GLN	engineered mutation	UNP P04585
A	280	SER	CYS	engineered mutation	UNP P04585

- Molecule 2 is a protein called Reverse transcriptase p51 subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	414	3411	2218	567	619	7	0	0	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	expression tag	UNP P04585
B	-10	GLY	-	expression tag	UNP P04585
B	-9	SER	-	expression tag	UNP P04585
B	-8	SER	-	expression tag	UNP P04585
B	-7	HIS	-	expression tag	UNP P04585
B	-6	HIS	-	expression tag	UNP P04585
B	-5	HIS	-	expression tag	UNP P04585
B	-4	HIS	-	expression tag	UNP P04585
B	-3	HIS	-	expression tag	UNP P04585
B	-2	HIS	-	expression tag	UNP P04585
B	-1	SER	-	expression tag	UNP P04585
B	0	SER	-	expression tag	UNP P04585
B	280	SER	CYS	engineered mutation	UNP P04585

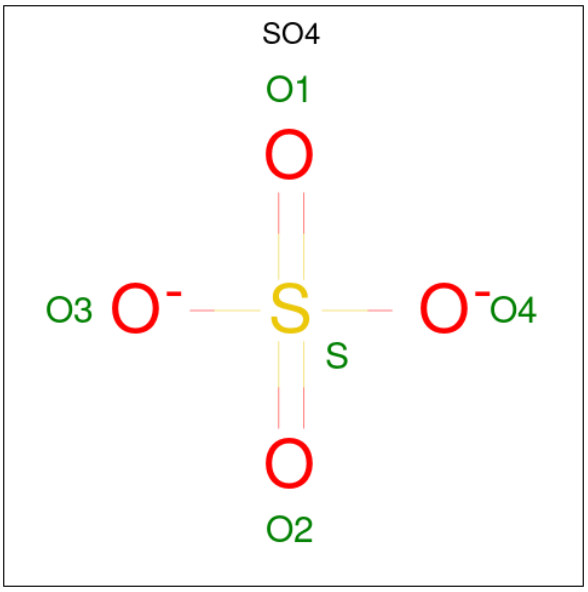
- Molecule 3 is a DNA chain called 5'-D(*AP*CP*A*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	P	18	360	172	62	109	17	0	0	0

- Molecule 4 is a DNA chain called 5'-D(*A*TP*GP*GP*TP*GP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	T	24	497	234	99	141	23	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

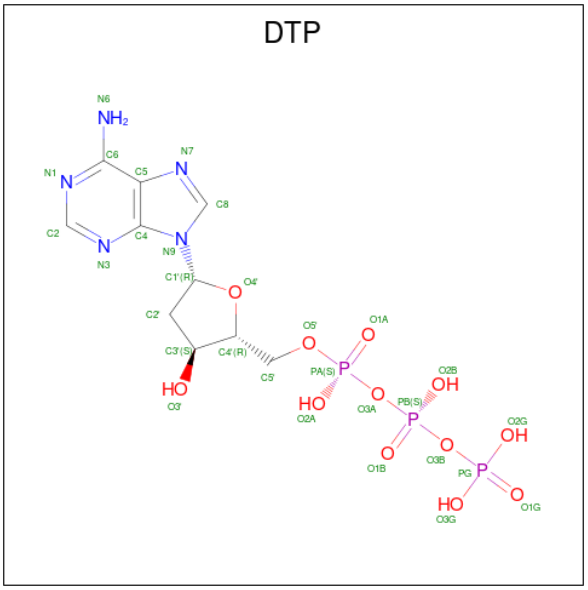


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	A	1	5	4	1	0	0
			Total	O	S		
5	P	1	5	4	1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	2	2	2	0	0

- Molecule 7 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
7	A	1	30	10	5	12	3	0	0

- Molecule 8 is water.

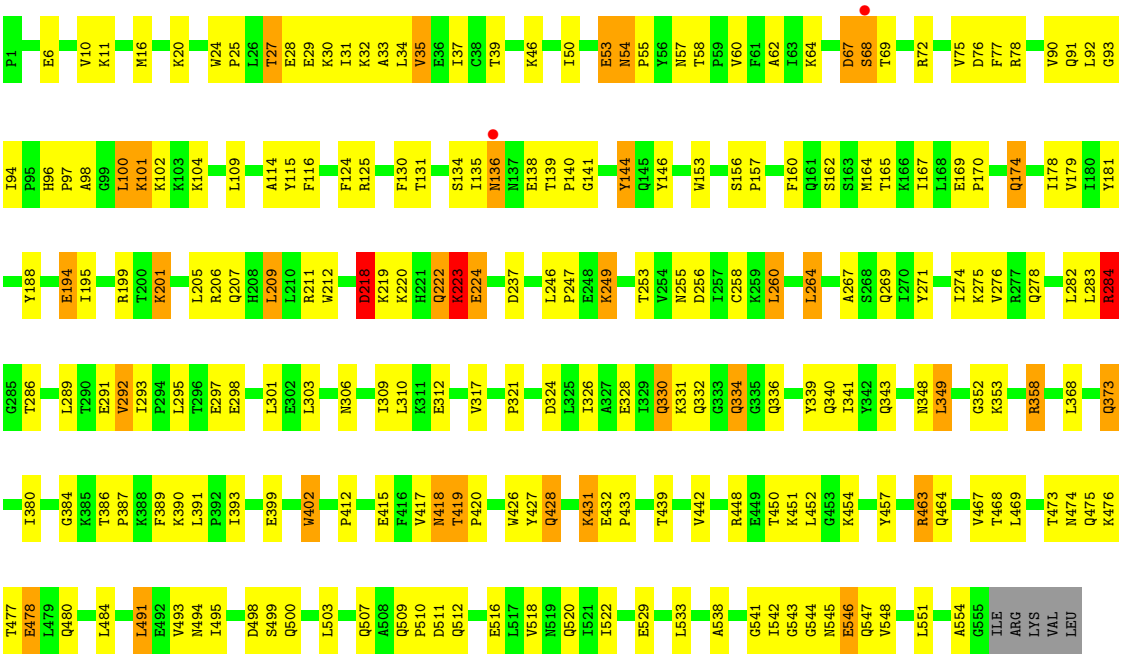
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	53	53	53	0	0
			Total	O		
8	B	29	29	29	0	0
			Total	O		
8	T	4	4	4	0	0

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.

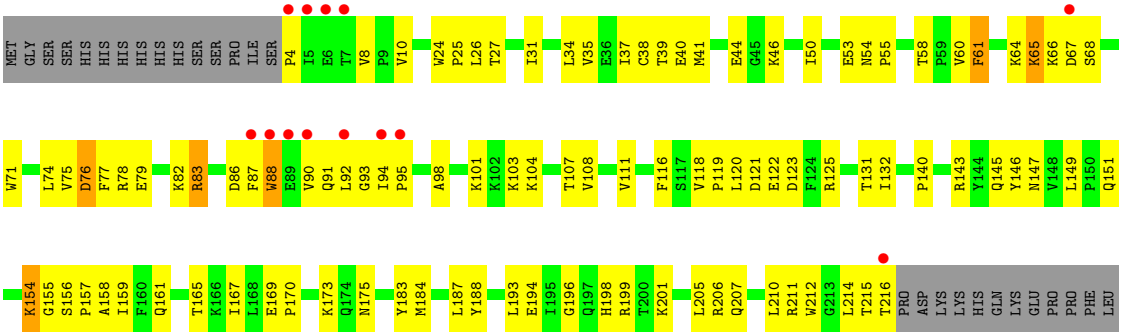
- Molecule 1: Reverse transcriptase p66 subunit

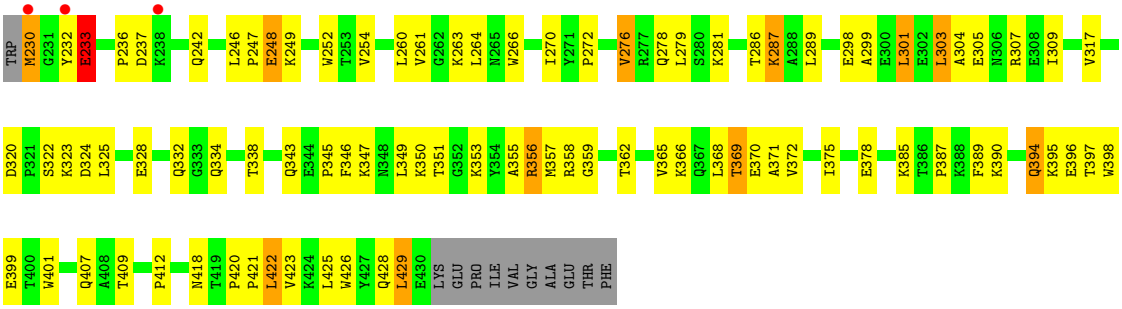
Chain A:



- Molecule 2: Reverse transcriptase p51 subunit

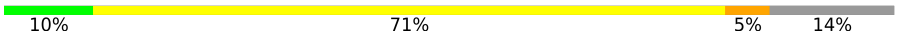
Chain B:

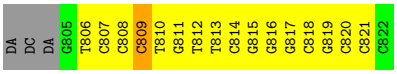




• Molecule 3: 5'-D(*AP*CP*A*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*(DOC))-3'

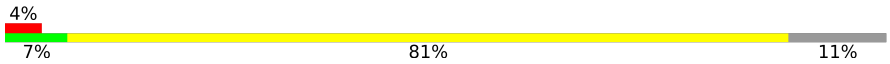
Chain P:

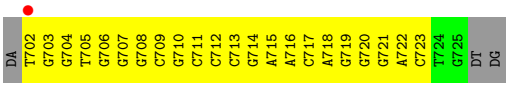




• Molecule 4: 5'-D(*A*TP*GP*GP*TP*GP*GP*GP*CP*GP*CP*CP*CP*GP*AP*AP*CP*AP*GP*GP*GP*AP*CP*TP*GP*TP*G)-3'

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	167.91Å 168.92Å 102.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.77 – 2.90 47.30 – 2.83	Depositor EDS
% Data completeness (in resolution range)	94.0 (29.77-2.90) 90.4 (47.30-2.83)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.09 (at 2.81Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.198 , 0.259 0.198 , 0.254	Depositor DCC
R_{free} test set	1519 reflections (4.49%)	wwPDB-VP
Wilson B-factor (Å^2)	50.9	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8915	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: DTP, SO4, DOC, 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	0.37	0/4631	0.55	0/6292
2	B	0.35	0/3506	0.54	1/4763 (0.0%)
3	P	0.47	0/381	1.11	1/586 (0.2%)
4	T	0.46	0/559	0.92	0/863
All	All	0.37	0/9077	0.61	2/12504 (0.0%)

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

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	4	PRO	N-CA-CB	5.33	109.70	103.30
3	P	809	DC	N1-C1'-C2'	5.10	122.30	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	TYR	Sidechain
1	A	218	ASP	Peptide
1	A	224	GLU	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	4514	0	4563	206	0
2	B	3411	0	3437	156	0
3	P	360	0	204	20	0
4	T	497	0	269	28	0
5	A	10	0	0	0	0
5	P	5	0	0	0	0
6	A	2	0	0	0	0
7	A	30	0	12	1	0
8	A	53	0	0	3	0
8	B	29	0	0	1	0
8	T	4	0	0	1	0
All	All	8915	0	8485	395	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 23.

All (395) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:THR:HG21	1:A:293:ILE:HD11	1.45	0.97
2:B:92:LEU:HD22	2:B:94:ILE:HD11	1.46	0.97
1:A:135:ILE:H	1:A:135:ILE:HD12	1.31	0.94
2:B:35:VAL:O	2:B:39:THR:HG23	1.74	0.86
2:B:94:ILE:HD12	2:B:94:ILE:H	1.41	0.85
1:A:431:LYS:H	1:A:431:LYS:HD3	1.45	0.81
1:A:97:PRO:HA	1:A:100:LEU:HD22	1.60	0.80
1:A:199:ARG:HG3	1:A:199:ARG:HH11	1.45	0.80
1:A:412:PRO:HG3	2:B:401:TRP:CZ2	2.16	0.80
2:B:65:LYS:HA	2:B:407:GLN:HE22	1.48	0.78
2:B:88:TRP:HB2	2:B:154:LYS:HE2	1.63	0.78
2:B:365:VAL:O	2:B:369:THR:HG23	1.84	0.78
1:A:199:ARG:NH2	1:A:223:LYS:HB2	1.98	0.78
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.65	0.77
1:A:134:SER:HB3	1:A:139:THR:HB	1.65	0.76
2:B:357:MET:HG2	2:B:359:GLY:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HD1	1:A:98:ALA:H	1.31	0.76
1:A:274:ILE:HD13	1:A:306:ASN:HD22	1.51	0.76
1:A:286:THR:HG21	1:A:293:ILE:CD1	2.15	0.75
2:B:278:GLN:OE1	2:B:298:GLU:HG3	1.87	0.75
1:A:253:THR:H	1:A:256:ASP:HB2	1.52	0.75
1:A:64:LYS:HD3	1:A:68:SER:O	1.87	0.74
1:A:218:ASP:OD1	1:A:218:ASP:N	2.19	0.74
1:A:428:GLN:HE21	1:A:428:GLN:HA	1.52	0.74
2:B:242:GLN:HE22	2:B:429:LEU:HD21	1.52	0.74
1:A:511:ASP:OD1	1:A:512:GLN:HG3	1.87	0.74
2:B:242:GLN:NE2	2:B:429:LEU:HD21	2.03	0.74
1:A:417:VAL:HG12	1:A:419:THR:HG22	1.70	0.73
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.70	0.73
2:B:66:LYS:CD	2:B:67:ASP:H	2.02	0.73
2:B:303:LEU:O	2:B:303:LEU:HD22	1.88	0.73
4:T:705:DT:H2"	4:T:706:DG:H5'	1.71	0.72
2:B:92:LEU:HD21	2:B:158:ALA:HA	1.71	0.72
1:A:222:GLN:O	1:A:224:GLU:N	2.22	0.71
1:A:541:GLY:HA2	1:A:546:GLU:HG2	1.70	0.71
1:A:516:GLU:O	1:A:520:GLN:HG3	1.91	0.71
1:A:199:ARG:HG3	1:A:199:ARG:NH1	2.05	0.70
1:A:57:ASN:OD1	1:A:131:THR:HG22	1.91	0.70
1:A:473:THR:OG1	1:A:476:LYS:HG3	1.91	0.70
4:T:712:DC:H2'	4:T:713:DC:C6	2.26	0.70
1:A:135:ILE:H	1:A:135:ILE:CD1	2.04	0.70
1:A:478:GLU:HG2	1:A:499:SER:HB2	1.73	0.70
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.74	0.69
2:B:125:ARG:HD3	2:B:146:TYR:O	1.92	0.69
1:A:27:THR:O	1:A:31:ILE:HG13	1.93	0.69
1:A:454:LYS:NZ	1:A:554:ALA:HB3	2.08	0.68
1:A:139:THR:HG22	1:A:141:GLY:CA	2.24	0.68
4:T:714:DG:H2'	4:T:715:DA:C8	2.28	0.68
1:A:358:ARG:NH1	1:A:358:ARG:HB3	2.10	0.67
1:A:478:GLU:HG2	1:A:499:SER:CB	2.24	0.67
2:B:93:GLY:O	2:B:95:PRO:HD3	1.95	0.67
1:A:53:GLU:O	1:A:55:PRO:HD3	1.95	0.67
1:A:97:PRO:HA	1:A:100:LEU:CD2	2.24	0.67
1:A:275:LYS:H	1:A:306:ASN:HD21	1.42	0.67
1:A:140:PRO:N	1:A:141:GLY:HA2	2.09	0.67
2:B:64:LYS:HE2	2:B:68:SER:O	1.95	0.67
1:A:518:VAL:O	1:A:522:ILE:HG13	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:334:GLN:O	2:B:358:ARG:HG2	1.94	0.67
1:A:218:ASP:HA	1:A:220:LYS:N	2.09	0.66
2:B:10:VAL:HG13	2:B:87:PHE:CZ	2.30	0.66
2:B:98:ALA:O	2:B:101:LYS:HG2	1.94	0.66
1:A:125:ARG:HG2	1:A:146:TYR:O	1.95	0.66
1:A:247:PRO:HD2	1:A:260:LEU:HD23	1.76	0.66
1:A:199:ARG:HH21	1:A:223:LYS:HB2	1.60	0.66
4:T:707:DG:H2"	4:T:708:DG:H5'	1.77	0.66
1:A:139:THR:HG22	1:A:141:GLY:HA2	1.77	0.66
2:B:103:LYS:O	2:B:236:PRO:HD2	1.96	0.66
2:B:425:LEU:HD13	2:B:425:LEU:O	1.96	0.66
1:A:20:LYS:NZ	1:A:55:PRO:HB2	2.10	0.66
2:B:249:LYS:HB2	2:B:252:TRP:CE2	2.31	0.65
2:B:26:LEU:HA	8:B:460:HOH:O	1.96	0.65
2:B:193:LEU:HD12	2:B:198:HIS:HA	1.78	0.64
2:B:61:PHE:CZ	2:B:74:LEU:HD23	2.31	0.64
3:P:817:DG:H2'	3:P:818:DC:C6	2.32	0.64
1:A:178:ILE:CD1	1:A:201:LYS:HG2	2.27	0.64
1:A:412:PRO:HG3	2:B:401:TRP:HZ2	1.60	0.64
2:B:334:GLN:HB3	2:B:358:ARG:HE	1.62	0.64
2:B:425:LEU:HA	2:B:428:GLN:HG3	1.80	0.64
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.79	0.64
1:A:332:GLN:HB2	1:A:336:GLN:HB2	1.80	0.64
3:P:813:DT:H2'	3:P:814:DC:C6	2.33	0.64
4:T:716:DA:H2'	4:T:717:DC:O4'	1.98	0.64
2:B:246:LEU:HD11	2:B:264:LEU:HD21	1.80	0.63
2:B:170:PRO:HA	2:B:173:LYS:HE3	1.79	0.63
1:A:454:LYS:HD3	1:A:468:THR:HG22	1.80	0.63
2:B:369:THR:HA	2:B:372:VAL:HG22	1.80	0.63
1:A:431:LYS:HG2	1:A:432:GLU:HG2	1.80	0.62
1:A:30:LYS:O	1:A:34:LEU:HG	1.98	0.62
1:A:249:LYS:HG2	1:A:256:ASP:OD2	1.99	0.62
1:A:96:HIS:CG	1:A:97:PRO:HD2	2.35	0.62
2:B:92:LEU:HB3	2:B:94:ILE:CD1	2.30	0.62
2:B:10:VAL:HG13	2:B:87:PHE:HZ	1.64	0.61
2:B:66:LYS:HD2	2:B:67:ASP:H	1.66	0.61
2:B:94:ILE:HD12	2:B:94:ILE:N	2.13	0.61
4:T:708:DG:H2'	4:T:709:DC:C6	2.35	0.61
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.83	0.61
1:A:454:LYS:CD	1:A:468:THR:HG22	2.30	0.61
1:A:544:GLY:HA3	2:B:286:THR:HG22	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ILE:HD12	1:A:135:ILE:N	2.10	0.61
2:B:65:LYS:HD3	2:B:407:GLN:NE2	2.16	0.60
1:A:27:THR:HG22	1:A:29:GLU:H	1.65	0.60
1:A:53:GLU:H	1:A:53:GLU:CD	2.03	0.60
1:A:93:GLY:C	1:A:94:ILE:HD13	2.20	0.60
1:A:358:ARG:HB3	1:A:358:ARG:HH11	1.64	0.60
1:A:475:GLN:NE2	3:P:808:DC:H2"	2.16	0.60
1:A:543:GLY:CA	1:A:546:GLU:HB2	2.32	0.60
1:A:495:ILE:O	1:A:533:LEU:HD12	2.00	0.59
2:B:120:LEU:HD22	2:B:121:ASP:N	2.18	0.59
1:A:448:ARG:HH12	3:P:807:DC:H1'	1.66	0.59
2:B:86:ASP:O	2:B:90:VAL:HB	2.03	0.59
2:B:423:VAL:HA	2:B:426:TRP:CD1	2.37	0.59
1:A:60:VAL:HG12	1:A:75:VAL:HG22	1.85	0.59
1:A:274:ILE:HD13	1:A:306:ASN:ND2	2.18	0.58
1:A:418:ASN:O	1:A:420:PRO:HD3	2.04	0.58
1:A:194:GLU:HB3	8:A:575:HOH:O	2.02	0.58
2:B:325:LEU:CD2	2:B:385:LYS:HD3	2.33	0.58
2:B:332:GLN:HA	2:B:332:GLN:OE1	2.03	0.58
2:B:357:MET:CE	2:B:359:GLY:HA3	2.33	0.58
2:B:155:GLY:O	2:B:159:ILE:HG12	2.04	0.57
1:A:109:LEU:CD2	1:A:220:LYS:HG3	2.34	0.57
1:A:473:THR:HG23	1:A:476:LYS:HD2	1.86	0.57
1:A:324:ASP:O	1:A:343:GLN:HG2	2.04	0.57
1:A:467:VAL:HG23	1:A:484:LEU:HD21	1.85	0.57
4:T:713:DC:H2'	4:T:714:DG:C8	2.39	0.57
1:A:96:HIS:NE2	1:A:269:GLN:NE2	2.52	0.57
1:A:380:ILE:O	1:A:384:GLY:HA2	2.04	0.57
2:B:27:THR:O	2:B:31:ILE:HD12	2.05	0.57
3:P:820:DC:H2"	3:P:821:DC:H5'	1.87	0.57
1:A:246:LEU:HD21	1:A:264:LEU:HD13	1.86	0.57
4:T:711:DC:H2'	4:T:712:DC:C6	2.39	0.57
1:A:27:THR:HG22	1:A:29:GLU:N	2.20	0.57
1:A:500:GLN:HG2	2:B:422:LEU:HD22	1.86	0.56
2:B:87:PHE:HA	2:B:91:GLN:HB2	1.86	0.56
1:A:50:ILE:HD12	1:A:54:ASN:CB	2.35	0.56
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.70	0.56
2:B:249:LYS:HB2	2:B:252:TRP:NE1	2.20	0.56
4:T:702:DT:H5"	8:T:38:HOH:O	2.04	0.56
1:A:417:VAL:CG1	1:A:419:THR:HG22	2.35	0.56
1:A:282:LEU:HD21	1:A:295:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:LEU:HD11	1:A:507:GLN:HE21	1.71	0.56
2:B:303:LEU:HD13	2:B:307:ARG:HH12	1.70	0.56
1:A:76:ASP:OD1	1:A:78:ARG:HG3	2.05	0.56
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.88	0.56
2:B:78:ARG:O	2:B:82:LYS:HG3	2.06	0.55
2:B:303:LEU:HD13	2:B:307:ARG:NH1	2.21	0.55
1:A:255:ASN:HB2	1:A:289:LEU:HG	1.87	0.55
2:B:120:LEU:HD22	2:B:121:ASP:H	1.70	0.55
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.88	0.55
2:B:369:THR:HG22	2:B:398:TRP:CZ3	2.42	0.55
1:A:50:ILE:HD12	1:A:54:ASN:HB3	1.87	0.55
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.89	0.55
1:A:547:GLN:O	1:A:551:LEU:HD13	2.07	0.55
2:B:79:GLU:HG3	2:B:83:ARG:NH1	2.22	0.55
2:B:394:GLN:OE1	2:B:396:GLU:HG2	2.06	0.55
1:A:303:LEU:HD12	1:A:303:LEU:O	2.07	0.55
1:A:195:ILE:HG12	8:A:591:HOH:O	2.08	0.54
1:A:255:ASN:HD22	1:A:289:LEU:CG	2.19	0.54
1:A:399:GLU:O	1:A:402:TRP:HD1	1.89	0.54
2:B:40:GLU:OE2	2:B:40:GLU:HA	2.08	0.54
2:B:58:THR:HG23	2:B:76:ASP:O	2.06	0.54
1:A:274:ILE:HA	1:A:306:ASN:ND2	2.22	0.54
1:A:260:LEU:O	1:A:264:LEU:HD22	2.07	0.54
2:B:65:LYS:HB2	2:B:65:LYS:NZ	2.23	0.54
1:A:543:GLY:HA2	1:A:546:GLU:H	1.73	0.54
2:B:131:THR:HG23	2:B:143:ARG:HG3	1.90	0.54
1:A:439:THR:CG2	2:B:289:LEU:HD13	2.38	0.54
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.48	0.54
1:A:115:TYR:CE2	1:A:156:SER:HB3	2.43	0.54
3:P:809:DC:H2"	3:P:810:DT:O5'	2.06	0.54
4:T:721:DG:H2"	4:T:722:DA:O5'	2.08	0.54
3:P:810:DT:H2'	3:P:811:DG:C8	2.43	0.53
1:A:306:ASN:HA	1:A:309:ILE:HG22	1.90	0.53
2:B:94:ILE:H	2:B:94:ILE:CD1	2.18	0.52
2:B:196:GLY:H	2:B:199:ARG:HG3	1.74	0.52
1:A:278:GLN:O	1:A:282:LEU:HD13	2.10	0.52
2:B:328:GLU:HG2	2:B:390:LYS:HD2	1.92	0.52
1:A:93:GLY:O	1:A:94:ILE:HD13	2.10	0.52
1:A:218:ASP:HA	1:A:220:LYS:H	1.73	0.52
1:A:433:PRO:HB3	2:B:289:LEU:HD23	1.92	0.52
2:B:66:LYS:HD3	2:B:67:ASP:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:LYS:HZ3	1:A:55:PRO:HB2	1.75	0.51
2:B:78:ARG:NH1	2:B:412:PRO:O	2.43	0.51
1:A:46:LYS:HD3	1:A:116:PHE:O	2.11	0.51
1:A:78:ARG:NH1	4:T:705:DT:H5"	2.25	0.51
2:B:34:LEU:HD11	2:B:61:PHE:HA	1.92	0.51
1:A:330:GLN:NE2	1:A:340:GLN:HE21	2.09	0.51
2:B:371:ALA:O	2:B:375:ILE:HG13	2.10	0.51
3:P:816:DG:H2'	3:P:817:DG:C8	2.46	0.51
2:B:323:LYS:O	2:B:385:LYS:HE2	2.09	0.51
4:T:721:DG:H2'	4:T:722:DA:C8	2.46	0.51
2:B:118:VAL:HG12	2:B:119:PRO:O	2.10	0.51
1:A:24:TRP:HB2	1:A:25:PRO:HD2	1.93	0.51
4:T:706:DG:H2'	4:T:707:DG:C8	2.46	0.51
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.76	0.50
1:A:253:THR:HG22	1:A:292:VAL:HB	1.93	0.50
1:A:101:LYS:CE	1:A:321:PRO:HG3	2.41	0.50
1:A:317:VAL:HG23	1:A:349:LEU:HD13	1.94	0.50
1:A:450:THR:O	1:A:452:LEU:HD13	2.11	0.50
4:T:720:DG:H2'	4:T:721:DG:C8	2.47	0.50
1:A:503:LEU:O	1:A:507:GLN:HG3	2.12	0.50
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.46	0.50
2:B:317:VAL:HG12	2:B:349:LEU:HD23	1.93	0.50
2:B:79:GLU:OE1	2:B:82:LYS:HE2	2.11	0.50
1:A:72:ARG:HA	8:A:568:HOH:O	2.11	0.50
2:B:320:ASP:OD1	2:B:320:ASP:C	2.50	0.50
1:A:199:ARG:HH11	1:A:199:ARG:CG	2.21	0.49
1:A:464:GLN:NE2	1:A:551:LEU:HD21	2.28	0.49
1:A:454:LYS:HZ2	1:A:554:ALA:HB3	1.76	0.49
1:A:27:THR:HG22	1:A:28:GLU:N	2.27	0.49
1:A:495:ILE:HB	1:A:533:LEU:HD13	1.94	0.49
1:A:317:VAL:HG22	1:A:348:ASN:O	2.12	0.49
2:B:53:GLU:OE1	2:B:53:GLU:N	2.34	0.49
2:B:395:LYS:O	2:B:399:GLU:HG3	2.13	0.49
1:A:334:GLN:CD	1:A:334:GLN:N	2.65	0.49
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.94	0.49
1:A:457:TYR:HA	1:A:548:VAL:HG21	1.93	0.49
2:B:61:PHE:N	2:B:61:PHE:CD1	2.81	0.49
1:A:246:LEU:HD11	1:A:310:LEU:HD12	1.93	0.49
2:B:260:LEU:HD23	2:B:279:LEU:HD22	1.94	0.49
4:T:710:DG:H2"	4:T:711:DC:H5'	1.94	0.49
1:A:139:THR:HG22	1:A:141:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:263:LYS:HE3	2:B:426:TRP:O	2.13	0.49
1:A:253:THR:HG22	1:A:292:VAL:HA	1.94	0.49
2:B:263:LYS:HA	2:B:426:TRP:CZ3	2.48	0.49
3:P:813:DT:H2"	3:P:814:DC:C5'	2.43	0.48
1:A:544:GLY:CA	2:B:286:THR:HG22	2.42	0.48
2:B:303:LEU:O	2:B:307:ARG:HB2	2.14	0.48
4:T:711:DC:H2'	4:T:712:DC:H6	1.78	0.48
3:P:810:DT:H2'	3:P:811:DG:H8	1.78	0.48
1:A:31:ILE:O	1:A:35:VAL:HG13	2.14	0.48
1:A:35:VAL:O	1:A:39:THR:HG23	2.14	0.48
2:B:44:GLU:OE2	2:B:46:LYS:HE3	2.12	0.48
4:T:718:DA:H2'	4:T:719:DG:O4'	2.12	0.48
1:A:439:THR:HG21	2:B:289:LEU:HD13	1.96	0.48
2:B:357:MET:O	2:B:362:THR:HG22	2.14	0.47
1:A:101:LYS:HE2	1:A:321:PRO:HG3	1.95	0.47
1:A:454:LYS:NZ	1:A:554:ALA:CB	2.75	0.47
1:A:464:GLN:O	1:A:464:GLN:HG3	2.13	0.47
1:A:542:ILE:O	1:A:545:ASN:HB3	2.14	0.47
4:T:702:DT:H2"	4:T:703:DG:O5'	2.14	0.47
1:A:165:THR:OG1	2:B:140:PRO:HG2	2.14	0.47
3:P:806:DT:H2'	3:P:807:DC:C6	2.49	0.47
4:T:709:DC:H2'	4:T:710:DG:H8	1.80	0.47
1:A:503:LEU:O	1:A:503:LEU:HG	2.13	0.47
2:B:26:LEU:HB2	2:B:31:ILE:HD11	1.96	0.47
2:B:65:LYS:HG2	2:B:230:MET:HG2	1.95	0.47
2:B:301:LEU:O	2:B:304:ALA:HB3	2.15	0.47
2:B:422:LEU:HG	2:B:426:TRP:CZ2	2.50	0.47
2:B:94:ILE:HG22	2:B:95:PRO:O	2.15	0.47
2:B:116:PHE:HZ	2:B:151:GLN:HE21	1.61	0.47
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.50	0.47
2:B:24:TRP:HB2	2:B:25:PRO:HD2	1.97	0.47
2:B:8:VAL:HG11	2:B:159:ILE:HG23	1.96	0.46
2:B:34:LEU:HA	2:B:34:LEU:HD23	1.66	0.46
2:B:175:ASN:OD1	2:B:201:LYS:HE3	2.14	0.46
3:P:808:DC:H2'	3:P:809:DC:C6	2.50	0.46
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.30	0.46
1:A:448:ARG:HG2	1:A:448:ARG:HH11	1.80	0.46
2:B:350:LYS:HE2	2:B:378:GLU:OE1	2.15	0.46
1:A:223:LYS:HA	1:A:223:LYS:HD2	1.76	0.46
2:B:261:VAL:HG13	2:B:276:VAL:CG2	2.44	0.46
1:A:426:TRP:O	1:A:427:TYR:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:GLU:HG3	2:B:83:ARG:HH11	1.80	0.46
4:T:705:DT:H2"	4:T:706:DG:C5'	2.43	0.46
1:A:10:VAL:HG23	1:A:124:PHE:CD1	2.50	0.46
2:B:214:LEU:HD12	2:B:215:THR:HG22	1.98	0.46
1:A:136:ASN:N	1:A:136:ASN:OD1	2.48	0.46
1:A:326:ILE:O	1:A:341:ILE:HA	2.15	0.46
1:A:493:VAL:HG22	1:A:494:ASN:N	2.31	0.46
2:B:353:LYS:HE2	2:B:429:LEU:HD13	1.98	0.46
1:A:67:ASP:C	1:A:69:THR:H	2.19	0.46
2:B:263:LYS:HA	2:B:426:TRP:CE3	2.50	0.46
1:A:135:ILE:HB	1:A:138:GLU:OE1	2.15	0.46
1:A:509:GLN:N	1:A:510:PRO:CD	2.78	0.46
3:P:817:DG:H2'	3:P:818:DC:H6	1.80	0.46
2:B:298:GLU:HG2	2:B:299:ALA:H	1.81	0.45
1:A:331:LYS:HG2	1:A:332:GLN:O	2.17	0.45
1:A:57:ASN:OD1	1:A:131:THR:CG2	2.64	0.45
1:A:67:ASP:O	1:A:69:THR:N	2.49	0.45
1:A:495:ILE:HB	1:A:533:LEU:CD1	2.47	0.45
1:A:33:ALA:O	1:A:37:ILE:HG13	2.17	0.45
1:A:417:VAL:O	1:A:419:THR:N	2.50	0.45
2:B:74:LEU:HD11	2:B:409:THR:HA	1.97	0.45
2:B:167:ILE:HG23	2:B:212:TRP:CE3	2.51	0.45
1:A:389:PHE:O	1:A:390:LYS:HD2	2.17	0.45
2:B:64:LYS:HD3	2:B:71:TRP:CE2	2.52	0.45
3:P:814:DC:H2'	3:P:815:DG:C8	2.51	0.45
3:P:815:DG:H2'	3:P:816:DG:C8	2.51	0.45
1:A:306:ASN:O	1:A:309:ILE:HG22	2.17	0.45
2:B:107:THR:HG23	2:B:232:TYR:HD1	1.82	0.45
2:B:120:LEU:CD1	2:B:125:ARG:HG2	2.46	0.45
2:B:254:VAL:HG21	2:B:287:LYS:HB2	1.98	0.45
3:P:813:DT:H2"	3:P:814:DC:H5'	1.98	0.45
3:P:818:DC:H2"	3:P:819:DG:H5'	1.98	0.45
1:A:167:ILE:HD13	1:A:212:TRP:HB3	1.99	0.44
2:B:76:ASP:OD1	2:B:76:ASP:C	2.56	0.44
2:B:108:VAL:HG22	2:B:188:TYR:CE2	2.52	0.44
1:A:306:ASN:HA	1:A:309:ILE:CG2	2.47	0.44
2:B:357:MET:HG2	2:B:359:GLY:N	2.26	0.44
1:A:264:LEU:O	1:A:267:ALA:HB3	2.17	0.44
1:A:274:ILE:HA	1:A:306:ASN:HD21	1.80	0.44
2:B:8:VAL:O	2:B:10:VAL:HG23	2.17	0.44
2:B:207:GLN:O	2:B:211:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:THR:HG21	1:A:77:PHE:CD1	2.52	0.44
2:B:149:LEU:HB3	2:B:156:SER:OG	2.18	0.44
2:B:357:MET:HE1	2:B:359:GLY:HA3	1.99	0.44
1:A:220:LYS:NZ	1:A:222:GLN:HG3	2.32	0.44
1:A:317:VAL:HG23	1:A:349:LEU:CD1	2.47	0.44
1:A:454:LYS:HZ1	1:A:554:ALA:CB	2.30	0.44
1:A:473:THR:O	1:A:477:THR:HG23	2.17	0.44
1:A:91:GLN:O	4:T:708:DG:H4'	2.18	0.44
1:A:271:TYR:CD1	1:A:310:LEU:HD23	2.52	0.44
4:T:709:DC:H2"	4:T:710:DG:H5'	2.00	0.44
2:B:320:ASP:H	2:B:343:GLN:HE22	1.66	0.44
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.99	0.44
2:B:355:ALA:O	2:B:356:ARG:HG2	2.18	0.44
1:A:253:THR:HG22	1:A:292:VAL:CB	2.48	0.43
1:A:393:ILE:HG23	1:A:393:ILE:O	2.17	0.43
2:B:214:LEU:HA	2:B:215:THR:HA	1.72	0.43
3:P:815:DG:H2'	3:P:816:DG:H8	1.83	0.43
1:A:10:VAL:HG11	1:A:153:TRP:HH2	1.83	0.43
1:A:140:PRO:CD	1:A:141:GLY:HA2	2.48	0.43
1:A:386:THR:HG23	1:A:387:PRO:HD2	2.01	0.43
1:A:391:LEU:HB2	1:A:393:ILE:HG22	2.00	0.43
1:A:246:LEU:CD1	1:A:310:LEU:HD12	2.48	0.43
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.54	0.43
2:B:122:GLU:O	2:B:125:ARG:HG3	2.19	0.43
1:A:543:GLY:HA2	1:A:546:GLU:N	2.33	0.43
2:B:165:THR:O	2:B:169:GLU:HB2	2.19	0.43
1:A:20:LYS:HZ1	1:A:55:PRO:HB2	1.82	0.43
1:A:255:ASN:HD22	1:A:289:LEU:CD1	2.31	0.43
1:A:373:GLN:NE2	2:B:397:THR:HG23	2.34	0.43
1:A:498:ASP:HB2	1:A:538:ALA:HB2	2.00	0.42
1:A:533:LEU:HD12	1:A:533:LEU:HA	1.81	0.42
7:A:563:DTP:H5'2	7:A:563:DTP:O1B	2.19	0.42
2:B:350:LYS:HG2	2:B:351:THR:N	2.34	0.42
2:B:366:LYS:O	2:B:370:GLU:HG3	2.19	0.42
1:A:101:LYS:HE2	1:A:321:PRO:CG	2.50	0.42
2:B:54:ASN:HA	2:B:55:PRO:HD3	1.78	0.42
4:T:721:DG:C2'	4:T:722:DA:O5'	2.68	0.42
1:A:543:GLY:HA2	1:A:545:ASN:N	2.34	0.42
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
2:B:201:LYS:HA	2:B:201:LYS:HD3	1.86	0.42
2:B:248:GLU:H	2:B:248:GLU:HG2	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:320:ASP:OD1	2:B:322:SER:N	2.51	0.42
4:T:709:DC:H2'	4:T:710:DG:C8	2.55	0.42
1:A:11:LYS:HB2	1:A:11:LYS:HE3	1.69	0.42
1:A:334:GLN:CD	1:A:334:GLN:H	2.22	0.42
2:B:125:ARG:HD3	2:B:147:ASN:HA	2.02	0.42
2:B:215:THR:OG1	2:B:216:THR:N	2.52	0.42
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.91	0.42
4:T:722:DA:H2'	4:T:723:DC:C6	2.55	0.42
1:A:195:ILE:O	1:A:199:ARG:HG2	2.20	0.42
1:A:431:LYS:H	1:A:431:LYS:CD	2.25	0.42
1:A:450:THR:O	1:A:451:LYS:HB2	2.20	0.42
2:B:156:SER:N	2:B:157:PRO:HD2	2.35	0.41
2:B:104:LYS:HB2	2:B:104:LYS:HE3	1.70	0.41
2:B:270:ILE:O	2:B:272:PRO:HD3	2.20	0.41
2:B:396:GLU:HG2	2:B:396:GLU:H	1.69	0.41
2:B:173:LYS:HE3	2:B:173:LYS:HB3	1.77	0.41
2:B:183:TYR:CE2	2:B:184:MET:HG2	2.55	0.41
3:P:811:DG:H2'	3:P:812:DT:C6	2.55	0.41
1:A:76:ASP:OD2	1:A:78:ARG:NH2	2.53	0.41
1:A:469:LEU:CD1	1:A:480:GLN:HG3	2.50	0.41
2:B:242:GLN:NE2	2:B:429:LEU:HD11	2.35	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.90	0.41
1:A:278:GLN:HG3	1:A:298:GLU:HB2	2.03	0.41
1:A:417:VAL:C	1:A:419:THR:H	2.23	0.41
2:B:121:ASP:OD1	2:B:121:ASP:C	2.58	0.41
2:B:420:PRO:C	2:B:422:LEU:H	2.23	0.41
3:P:812:DT:H2"	3:P:813:DT:C5'	2.50	0.41
1:A:135:ILE:HG21	1:A:138:GLU:OE2	2.20	0.41
1:A:439:THR:HG23	2:B:289:LEU:HD13	2.03	0.41
1:A:297:GLU:O	1:A:301:LEU:HD23	2.21	0.41
1:A:195:ILE:H	1:A:195:ILE:HG13	1.60	0.41
1:A:454:LYS:HZ1	1:A:554:ALA:HB3	1.81	0.41
2:B:266:TRP:CZ3	2:B:426:TRP:HB3	2.56	0.41
1:A:62:ALA:HA	1:A:72:ARG:O	2.21	0.41
1:A:102:LYS:HE2	1:A:237:ASP:OD1	2.20	0.41
1:A:463:ARG:H	1:A:463:ARG:HG2	1.61	0.41
2:B:345:PRO:O	2:B:346:PHE:HB2	2.21	0.41
4:T:710:DG:H2'	4:T:711:DC:C6	2.56	0.41
1:A:276:VAL:HG22	1:A:353:LYS:HE3	2.02	0.40
2:B:37:ILE:O	2:B:41:MET:HG3	2.21	0.40
1:A:178:ILE:HD11	1:A:201:LYS:HG2	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:PRO:O	2:B:307:ARG:NH2	2.54	0.40
1:A:90:VAL:O	1:A:92:LEU:HD13	2.22	0.40
2:B:232:TYR:O	2:B:233:GLU:HB2	2.22	0.40
4:T:703:DG:H2'	4:T:704:DG:C2	2.57	0.40
1:A:179:VAL:O	1:A:179:VAL:HG13	2.21	0.40
1:A:174:GLN:HE21	1:A:174:GLN:HB3	1.67	0.40
1:A:284:ARG:HG3	4:T:714:DG:OP1	2.21	0.40
1:A:328:GLU:O	1:A:339:TYR:HA	2.21	0.40
1:A:491:LEU:HB3	1:A:529:GLU:HG3	2.04	0.40
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.57	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	553/560 (99%)	517 (94%)	29 (5%)	7 (1%)	12	37
2	B	410/452 (91%)	372 (91%)	35 (8%)	3 (1%)	22	54
All	All	963/1012 (95%)	889 (92%)	64 (7%)	10 (1%)	15	45

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	LYS
2	B	233	GLU
1	A	284	ARG
1	A	418	ASN
2	B	88	TRP
1	A	291	GLU
1	A	27	THR
1	A	334	GLN

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Mol	Chain	Res	Type
1	A	68	SER
2	B	76	ASP

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	495/500 (99%)	447 (90%)	48 (10%)	8 25
2	B	373/411 (91%)	344 (92%)	29 (8%)	12 34
All	All	868/911 (95%)	791 (91%)	77 (9%)	9 29

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	16	MET
1	A	32	LYS
1	A	35	VAL
1	A	53	GLU
1	A	54	ASN
1	A	67	ASP
1	A	100	LEU
1	A	101	LYS
1	A	104	LYS
1	A	136	ASN
1	A	162	SER
1	A	164	MET
1	A	174	GLN
1	A	194	GLU
1	A	201	LYS
1	A	205	LEU
1	A	206	ARG
1	A	207	GLN
1	A	209	LEU
1	A	211	ARG

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Mol	Chain	Res	Type
1	A	218	ASP
1	A	219	LYS
1	A	222	GLN
1	A	223	LYS
1	A	249	LYS
1	A	258	CYS
1	A	260	LEU
1	A	264	LEU
1	A	283	LEU
1	A	284	ARG
1	A	292	VAL
1	A	312	GLU
1	A	330	GLN
1	A	349	LEU
1	A	358	ARG
1	A	368	LEU
1	A	373	GLN
1	A	402	TRP
1	A	415	GLU
1	A	419	THR
1	A	428	GLN
1	A	431	LYS
1	A	463	ARG
1	A	474	ASN
1	A	478	GLU
1	A	491	LEU
1	A	546	GLU
2	B	61	PHE
2	B	65	LYS
2	B	77	PHE
2	B	83	ARG
2	B	123	ASP
2	B	154	LYS
2	B	161	GLN
2	B	194	GLU
2	B	205	LEU
2	B	206	ARG
2	B	210	LEU
2	B	230	MET
2	B	233	GLU
2	B	237	ASP
2	B	248	GLU

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Mol	Chain	Res	Type
2	B	276	VAL
2	B	281	LYS
2	B	287	LYS
2	B	301	LEU
2	B	303	LEU
2	B	324	ASP
2	B	347	LYS
2	B	356	ARG
2	B	368	LEU
2	B	369	THR
2	B	394	GLN
2	B	418	ASN
2	B	422	LEU
2	B	429	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	161	GLN
1	A	174	GLN
1	A	175	ASN
1	A	197	GLN
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	269	GLN
1	A	306	ASN
1	A	330	GLN
1	A	332	GLN
1	A	428	GLN
1	A	464	GLN
1	A	474	ASN
1	A	480	GLN
2	B	91	GLN
2	B	147	ASN
2	B	182	GLN
2	B	197	GLN
2	B	207	GLN
2	B	242	GLN
2	B	278	GLN
2	B	343	GLN

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Mol	Chain	Res	Type
2	B	407	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)

1 non-standard protein/DNA/RNA residue is 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	$\#\|Z\| > 2$
3	DOC	P	822	4,3	16,19,20	0.44	0	20,26,29	0.49	0

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
3	DOC	P	822	4,3	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	SO4	A	561	-	4,4,4	0.26	0	6,6,6	0.09	0
7	DTP	A	563	6	26,32,32	1.01	1 (3%)	30,50,50	1.86	6 (20%)
5	SO4	A	562	-	4,4,4	0.29	0	6,6,6	0.11	0
5	SO4	P	2	-	4,4,4	0.28	0	6,6,6	0.09	0

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	DTP	A	563	6	-	6/18/34/34	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	563	DTP	C8-N7	-2.38	1.30	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	563	DTP	PB-O3B-PG	-5.32	114.57	132.83
7	A	563	DTP	N3-C2-N1	-4.54	121.58	128.68
7	A	563	DTP	PA-O3A-PB	-4.50	117.39	132.83
7	A	563	DTP	C2'-C1'-N9	-3.61	105.95	114.27
7	A	563	DTP	C4-C5-N7	-2.15	107.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	563	DTP	PA-O5'-C5'	-2.06	109.60	121.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	563	DTP	O4'-C4'-C5'-O5'
7	A	563	DTP	PB-O3B-PG-O1G
7	A	563	DTP	C3'-C4'-C5'-O5'
7	A	563	DTP	PB-O3B-PG-O2G
7	A	563	DTP	PB-O3B-PG-O3G
7	A	563	DTP	PA-O3A-PB-O1B

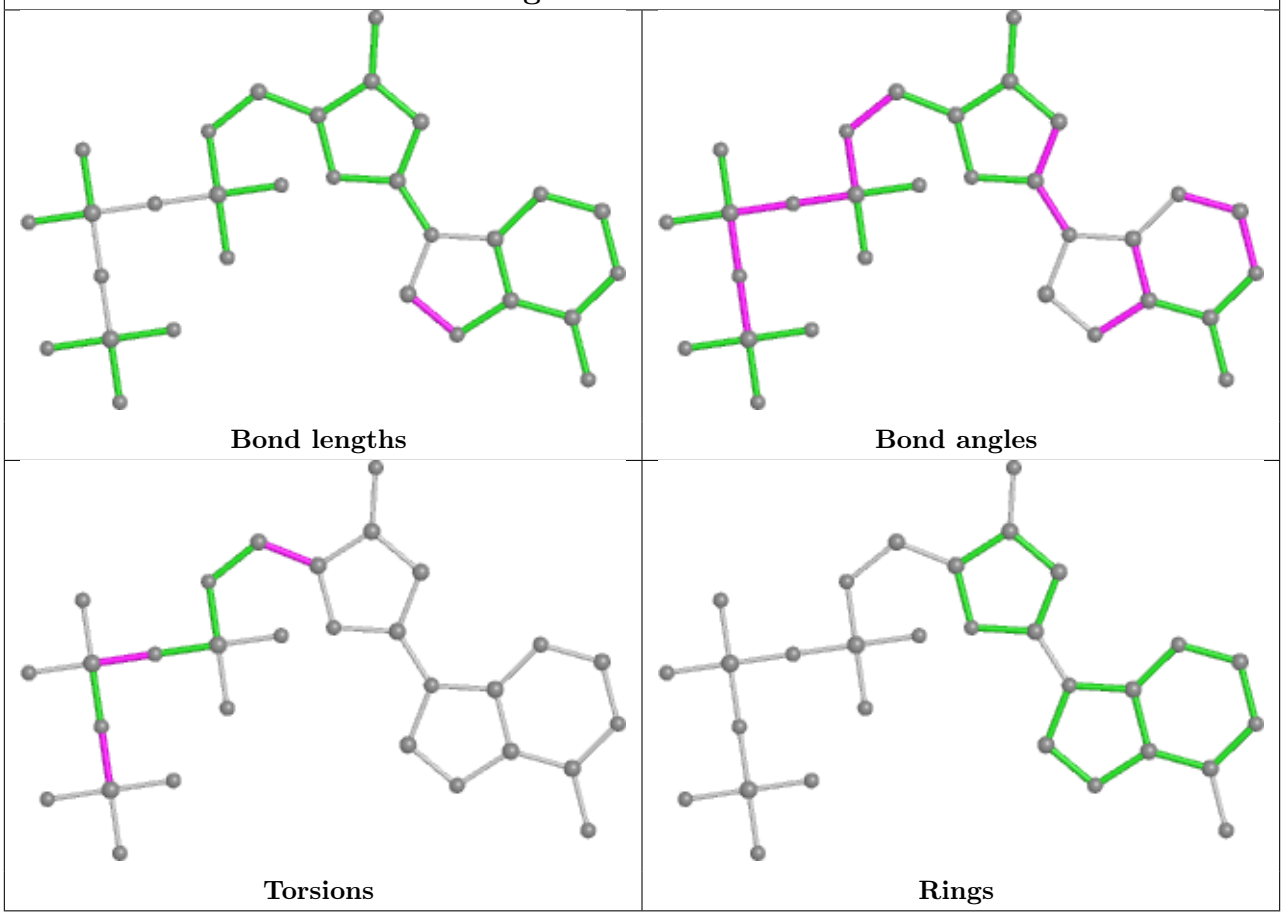
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	563	DTP	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 DTP A 563



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	555/560 (99%)	-0.34	2 (0%) 92 93	19, 38, 73, 101	0
2	B	414/452 (91%)	-0.08	16 (3%) 39 35	19, 52, 97, 121	0
3	P	17/21 (80%)	-0.57	0 100 100	32, 49, 65, 68	0
4	T	24/27 (88%)	-0.17	1 (4%) 36 32	32, 65, 98, 121	0
All	All	1010/1060 (95%)	-0.23	19 (1%) 66 65	19, 44, 88, 121	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	7.0
2	B	89	GLU	5.2
2	B	4	PRO	5.2
2	B	6	GLU	4.4
2	B	216	THR	3.6
2	B	5	ILE	3.3
1	A	136	ASN	3.1
2	B	230	MET	3.1
2	B	92	LEU	2.7
2	B	238	LYS	2.6
2	B	90	VAL	2.5
1	A	68	SER	2.5
2	B	94	ILE	2.5
2	B	87	PHE	2.4
2	B	95	PRO	2.1
2	B	232	TYR	2.1
2	B	67	ASP	2.1
4	T	702	DT	2.1
2	B	7	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
3	DOC	P	822	18/19	0.97	0.16	24,28,31,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

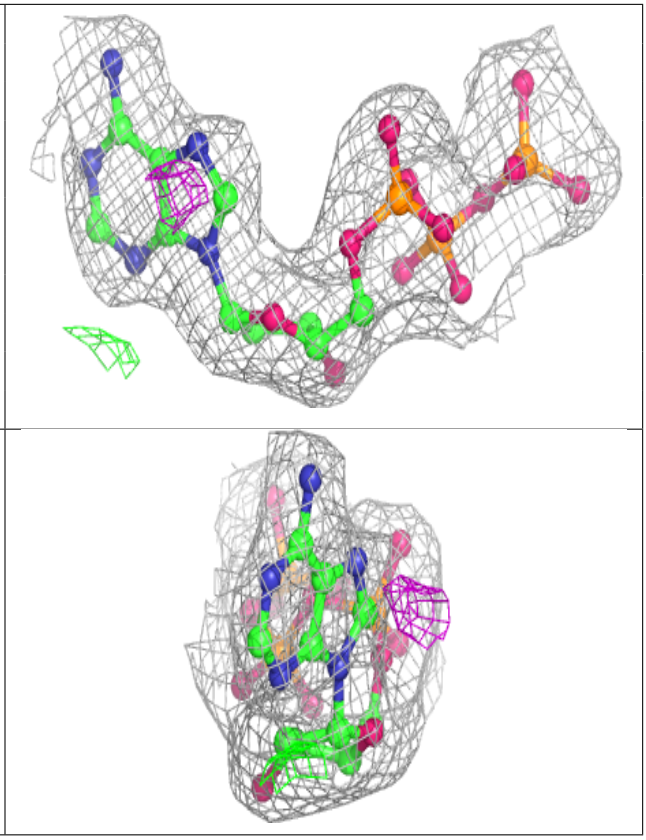
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	P	2	5/5	0.79	0.34	119,119,120,120	0
5	SO4	A	562	5/5	0.94	0.10	92,92,93,93	0
5	SO4	A	561	5/5	0.95	0.17	89,89,90,90	0
6	MG	A	600	1/1	0.96	0.09	5,5,5,5	0
7	DTP	A	563	30/30	0.97	0.14	25,36,43,44	0
6	MG	A	601	1/1	0.98	0.23	1,1,1,1	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 DTP A 563:

$2mF_o$-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.