



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 08:23 am BST

PDB ID : 4X0P
Title : Ternary complex of human DNA polymerase theta C-terminal domain binding ddATP opposite a tetrahydrofuran AP site analog
Authors : Zahn, K.E.; Doublet, S.
Deposited on : 2014-11-21
Resolution : 3.91 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

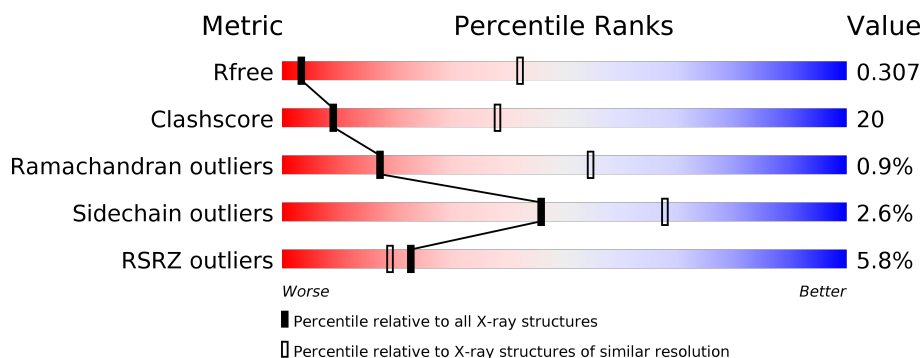
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.91 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.



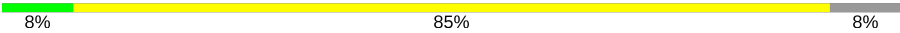
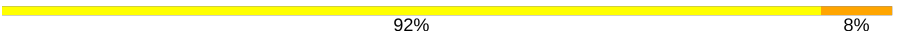
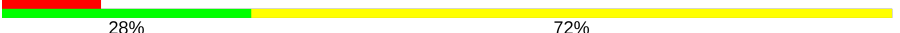



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RSRZ outliers	127900	1002 (4.20-3.64)

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 on 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	799	<div> <div>3%</div> <div> <div>47%</div> <div>29%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	799	<div> <div>4%</div> <div> <div>44%</div> <div>32%</div> <div>•</div> <div>22%</div> </div> </div>
1	C	799	<div> <div>6%</div> <div> <div>48%</div> <div>29%</div> <div>•</div> <div>22%</div> </div> </div>
1	D	799	<div> <div>6%</div> <div> <div>49%</div> <div>27%</div> <div>•</div> <div>22%</div> </div> </div>
2	F	13	<div> <div>23%</div> <div>69%</div> <div>8%</div> </div>
2	H	13	<div> <div>85%</div> <div>15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	13	
2	L	13	
3	E	18	
3	G	18	
3	I	18	
3	K	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	2601	-	-	-	X
4	GOL	A	2602	-	-	-	X
4	GOL	B	2601	-	-	-	X
4	GOL	C	2601	-	-	-	X
4	GOL	D	2601	-	-	-	X
6	DDS	B	2604	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 22448 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 polymerase theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			4963	3157	848	929	29			
1	B	625	Total	C	N	O	S	0	0	0
			4963	3157	848	929	29			
1	C	625	Total	C	N	O	S	0	0	0
			4963	3157	848	929	29			
1	D	625	Total	C	N	O	S	0	0	0
			4963	3157	848	929	29			

- Molecule 2 is a DNA chain called DNA (5'-D(P*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	12	Total	C	N	O	P	0	0	0
			243	116	40	75	12			
2	H	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			
2	J	12	Total	C	N	O	P	0	0	0
			243	116	40	75	12			
2	L	13	Total	C	N	O	P	0	0	0
			262	126	45	79	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	18	Total	C	N	O	P	0	0	0
			341	160	64	100	17			
3	G	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			
3	I	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	18	Total	C	N	O	P	0	0	0
			359	170	69	103	17			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

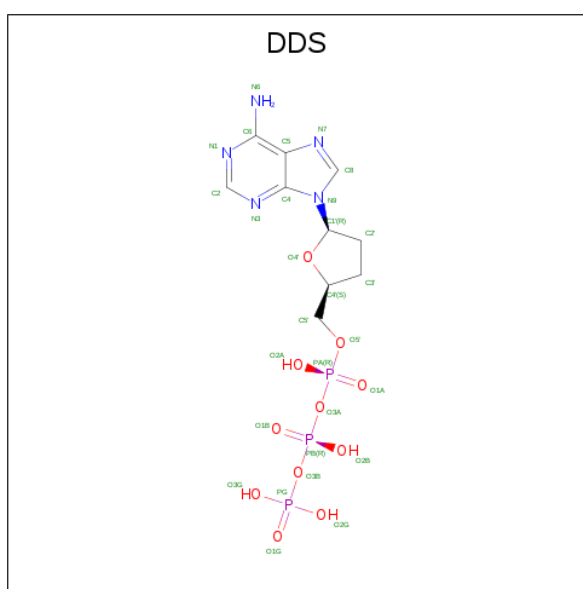


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

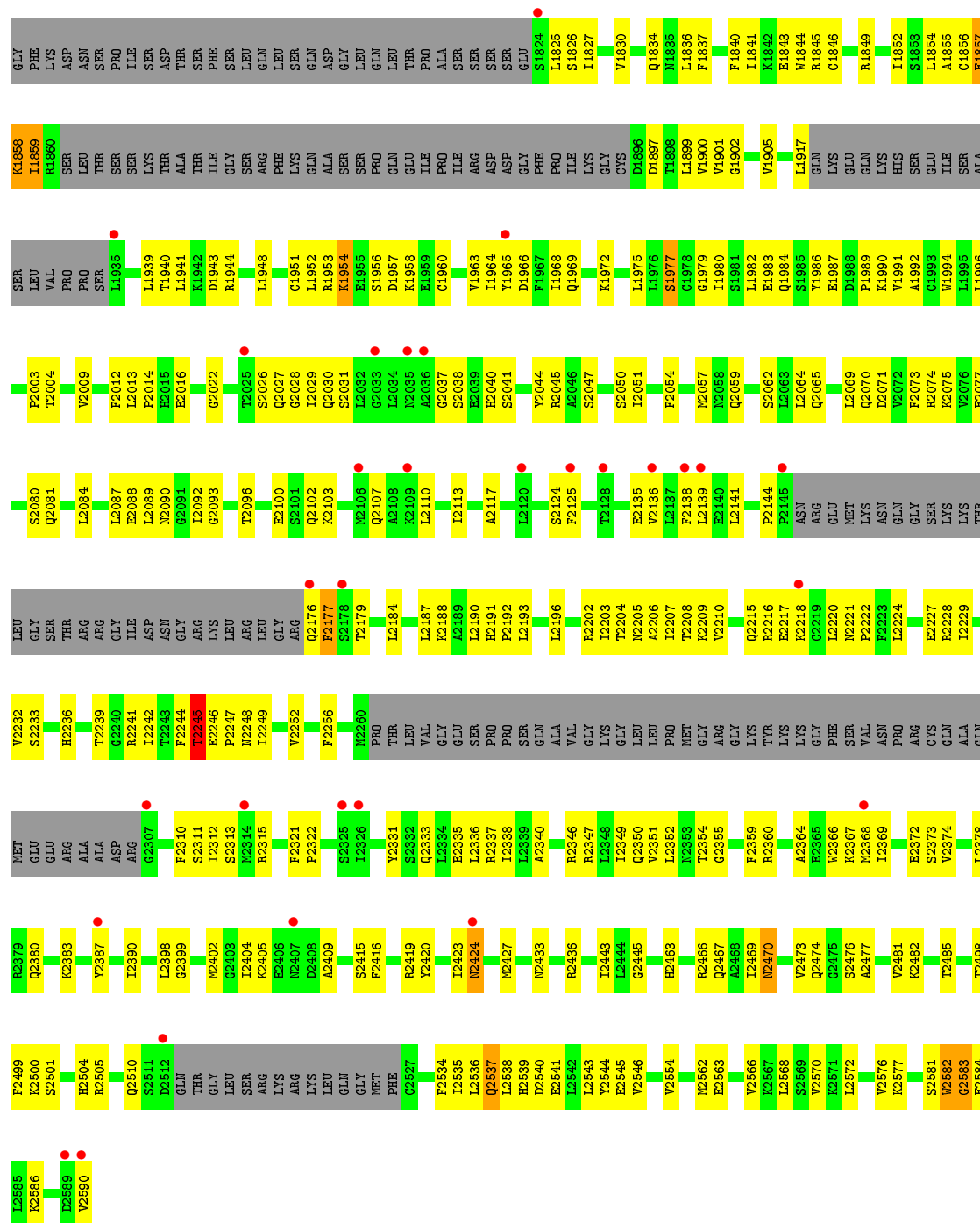
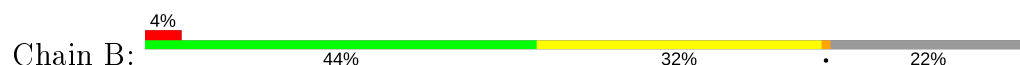
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Ca 1 1	0	0
5	A	1	Total Ca 1 1	0	0
5	D	1	Total Ca 1 1	0	0
5	C	1	Total Ca 1 1	0	0

- Molecule 6 is 2',3'-dideoxyadenosine triphosphate (three-letter code: DDS) (formula: $C_{10}H_{16}N_5O_{11}P_3$).



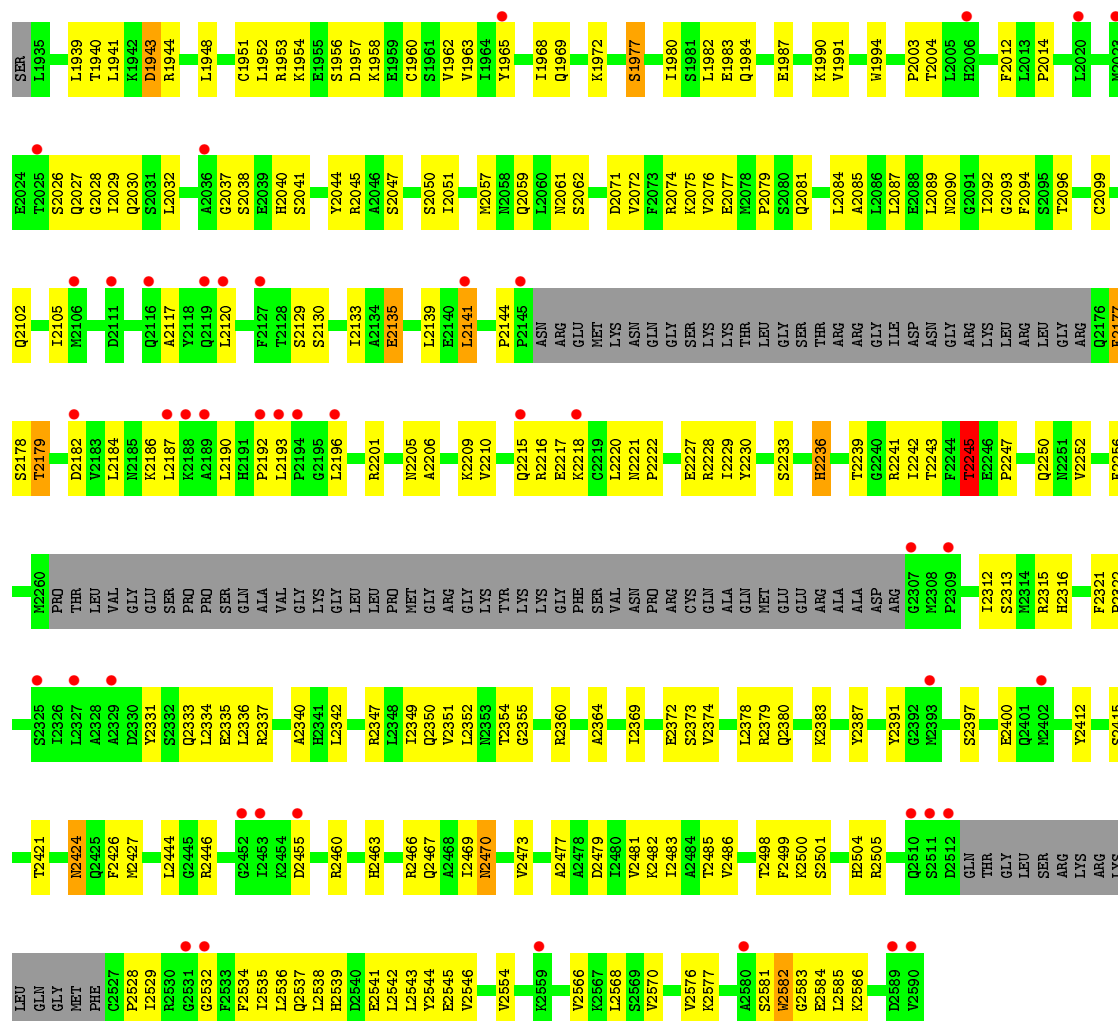


• Molecule 1: DNA polymerase theta



• Molecule 1: DNA polymerase theta





- Molecule 2: DNA (5'-D(P*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*C)-3')

Chain F: 23% 69% 8%



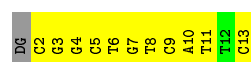
- Molecule 2: DNA (5'-D(P*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*C)-3')

Chain H: 85% 15%



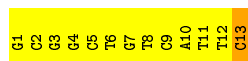
- Molecule 2: DNA (5'-D(P*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*C)-3')

Chain J: 8% 85% 8%



- Molecule 2: DNA (5'-D(P*CP*GP*GP*CP*TP*GP*TP*CP*AP*TP*TP*C)-3')

Chain L:  92% 8%



- Molecule 3: DNA (5'-D(*CP*GP*TP*TP*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain E:  11% 28% 72%



- Molecule 3: DNA (5'-D(*CP*GP*TP*TP*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain G:  28% 56% 17%



- Molecule 3: DNA (5'-D(*CP*GP*TP*TP*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain I:  33% 61% 6%



- Molecule 3: DNA (5'-D(*CP*GP*TP*TP*GP*AP*AP*TP*GP*AP*CP*AP*GP*CP*CP*GP*CP*G)-3')

Chain K:  50% 50%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	126.92Å 136.97Å 247.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.99 – 3.91 48.70 – 3.91	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.99-3.91) 99.2 (48.70-3.91)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.241 , 0.302 0.248 , 0.307	Depositor DCC
R_{free} test set	2005 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	149.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 130.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	22448	wwPDB-VP
Average B, all atoms (Å ²)	194.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DDS, GOL, CA

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	0/5056	0.67	0/6818
1	B	0.37	0/5056	0.67	0/6818
1	C	0.35	0/5056	0.66	0/6818
1	D	0.35	0/5056	0.64	0/6818
2	F	0.92	0/270	1.22	3/414 (0.7%)
2	H	0.90	0/292	1.15	2/449 (0.4%)
2	J	0.98	0/270	1.13	0/414
2	L	0.85	0/292	1.16	1/449 (0.2%)
3	E	0.83	0/382	1.01	0/588
3	G	0.79	0/403	1.08	3/620 (0.5%)
3	I	0.91	1/403 (0.2%)	0.94	0/620
3	K	0.82	0/403	1.06	0/620
All	All	0.45	1/22939 (0.0%)	0.73	9/31446 (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	5
1	B	0	4
1	C	0	4
1	D	0	4
All	All	0	17

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	10	DA	N9-C4	5.63	1.41	1.37

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2	DC	O4'-C1'-N1	7.28	113.09	108.00
2	L	13	DC	O4'-C1'-N1	7.26	113.08	108.00
3	G	9	DG	O4'-C1'-N9	-6.53	103.43	108.00
2	H	8	DT	O4'-C1'-N1	5.53	111.87	108.00
2	H	13	DC	O4'-C1'-N1	5.52	111.86	108.00
2	F	2	DC	O4'-C1'-C2'	5.46	110.27	105.90
3	G	1	DC	OP1-P-O3'	5.38	117.04	105.20
3	G	12	DA	O4'-C1'-N9	5.12	111.58	108.00
2	F	7	DG	O4'-C1'-N9	5.07	111.55	108.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1825	LEU	Peptide
1	A	1953	ARG	Peptide
1	A	2179	THR	Peptide
1	A	2245	THR	Peptide
1	A	2583	GLY	Peptide
1	B	1953	ARG	Peptide
1	B	2179	THR	Peptide
1	B	2245	THR	Peptide
1	B	2583	GLY	Peptide
1	C	1953	ARG	Peptide
1	C	2179	THR	Peptide
1	C	2245	THR	Peptide
1	C	2583	GLY	Peptide
1	D	1953	ARG	Peptide
1	D	2179	THR	Peptide
1	D	2245	THR	Peptide
1	D	2583	GLY	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4963	0	4980	193	1
1	B	4963	0	4980	218	0
1	C	4963	0	4980	187	0
1	D	4963	0	4980	176	0
2	F	243	0	137	10	0
2	H	262	0	149	24	0
2	J	243	0	137	21	0
2	L	262	0	149	23	0
3	E	341	0	185	21	0
3	G	359	0	197	29	0
3	I	359	0	197	19	0
3	K	359	0	197	24	1
4	A	12	0	16	0	0
4	B	12	0	16	1	0
4	C	12	0	16	0	0
4	D	12	0	16	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	1	0
5	D	1	0	0	0	0
6	A	29	0	12	4	0
6	B	29	0	12	9	0
6	C	29	0	12	4	0
6	D	29	0	12	6	0
All	All	22448	0	21380	880	1

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 20.

All (880) 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:C:2215:GLN:HA	1:C:2218:LYS:HE3	1.47	0.96
1:D:2499:PHE:HZ	1:D:2505:ARG:HE	1.11	0.96
1:B:2215:GLN:HA	1:B:2218:LYS:HE3	1.50	0.93
1:A:2499:PHE:HZ	1:A:2505:ARG:HE	1.19	0.90
1:C:2004:THR:HB	1:C:2026:SER:HB3	1.51	0.90
1:B:2499:PHE:HZ	1:B:2505:ARG:HE	1.18	0.89
1:A:2004:THR:HB	1:A:2026:SER:HB3	1.55	0.88
1:A:2215:GLN:HA	1:A:2218:LYS:HE3	1.56	0.88
1:C:2499:PHE:HZ	1:C:2505:ARG:HE	1.23	0.87
1:B:2004:THR:HB	1:B:2026:SER:HB3	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:13:DG:H2''	3:I:14:DC:H5''	1.57	0.86
3:E:10:DA:H2''	3:E:11:DC:H5'	1.55	0.86
1:B:2209:LYS:NZ	3:G:9:DG:N3	2.24	0.85
2:H:8:DT:H2''	2:H:9:DC:H5''	1.58	0.83
1:D:2215:GLN:HA	1:D:2218:LYS:HE3	1.59	0.83
1:B:2581:SER:OG	1:B:2582:TRP:N	2.11	0.82
1:D:2333:GLN:HB3	1:D:2336:LEU:HD12	1.59	0.81
2:J:8:DT:H2''	2:J:9:DC:H5'	1.60	0.81
1:B:2427:MET:HG3	1:B:2469:ILE:HD11	1.62	0.81
2:J:7:DG:H2''	2:J:8:DT:H5''	1.62	0.81
2:J:3:DG:O6	3:I:14:DC:N4	2.15	0.80
1:C:2581:SER:OG	1:C:2582:TRP:N	2.13	0.80
1:C:2315:ARG:HB2	1:C:2582:TRP:CD1	2.17	0.80
1:D:2315:ARG:HB2	1:D:2582:TRP:CD1	2.18	0.79
1:D:2004:THR:HB	1:D:2026:SER:HB3	1.64	0.78
1:B:2315:ARG:HB2	1:B:2582:TRP:CD1	2.19	0.78
1:C:1968:ILE:HD13	1:C:2233:SER:HB3	1.67	0.77
1:A:1963:VAL:HG12	1:A:1987:GLU:HB2	1.66	0.76
1:B:2030:GLN:O	1:B:2045:ARG:NH1	2.17	0.76
1:C:2383:LYS:NZ	6:C:2604:DDS:O2G	2.17	0.76
1:D:2374:VAL:HG13	1:D:2378:LEU:HD23	1.67	0.76
1:A:2084:LEU:HD11	1:A:2242:ILE:HD13	1.68	0.76
1:B:2037:GLY:O	1:B:2041:SER:N	2.19	0.76
2:F:4:DG:H2''	2:F:5:DC:H5''	1.67	0.75
1:A:2315:ARG:HB2	1:A:2582:TRP:CD1	2.21	0.75
3:I:5:DG:H2'	3:I:6:DA:C8	2.20	0.75
1:B:1948:LEU:HD22	1:B:1980:ILE:HD13	1.66	0.75
1:C:2084:LEU:HD11	1:C:2242:ILE:HD13	1.68	0.75
1:C:2337:ARG:HG2	1:C:2352:LEU:HD21	1.68	0.75
3:K:5:DG:H2'	3:K:6:DA:C8	2.22	0.74
3:E:9:DG:H2''	3:E:10:DA:H5''	1.67	0.74
1:C:2209:LYS:HE3	3:I:9:DG:H21	1.52	0.74
1:A:1960:CYS:SG	1:A:1984:GLN:NE2	2.60	0.73
1:C:2187:LEU:HA	1:C:2194:PRO:HG2	1.71	0.73
1:D:2205:ASN:OD1	1:D:2209:LYS:HD2	1.88	0.73
2:L:9:DC:H42	3:K:9:DG:H1	1.35	0.73
1:B:2337:ARG:HG2	1:B:2352:LEU:HD21	1.70	0.73
1:A:2093:GLY:HA2	1:A:2228:ARG:HG2	1.69	0.72
2:J:9:DC:H2''	2:J:10:DA:H5''	1.68	0.72
1:A:2337:ARG:HG2	1:A:2352:LEU:HD21	1.70	0.72
1:D:2581:SER:OG	1:D:2582:TRP:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:4:DG:H2''	2:J:5:DC:H5''	1.69	0.72
1:B:2568:LEU:HD12	1:B:2570:VAL:H	1.55	0.72
1:A:2201:ARG:NH2	2:F:10:DA:OP1	2.23	0.72
3:G:12:DA:H2''	3:G:13:DG:C8	2.26	0.71
1:C:1965:TYR:HB3	1:C:2029:ILE:HG22	1.71	0.71
1:C:2180:SER:HB2	2:J:10:DA:OP2	1.91	0.71
1:C:2540:ASP:OD1	5:C:2603:CA:CA	1.67	0.71
1:A:2374:VAL:HG13	1:A:2378:LEU:HD23	1.71	0.70
3:I:4:DT:H2'	3:I:5:DG:C8	2.26	0.70
1:A:2581:SER:OG	1:A:2582:TRP:N	2.25	0.70
3:E:5:DG:H2'	3:E:6:DA:C8	2.27	0.70
2:L:8:DT:H2''	2:L:9:DC:H5'	1.72	0.70
1:D:1965:TYR:HB3	1:D:2029:ILE:HG22	1.74	0.70
1:A:2193:LEU:HG	1:A:2196:LEU:HD13	1.74	0.69
1:D:1897:ASP:O	1:D:1977:SER:OG	2.10	0.69
1:D:2037:GLY:O	1:D:2041:SER:N	2.25	0.69
3:I:16:DG:H1'	3:I:17:DC:H5'	1.72	0.69
1:A:2383:LYS:NZ	6:A:2604:DDS:O2G	2.19	0.69
1:B:2041:SER:HA	1:B:2045:ARG:HE	1.55	0.69
1:D:2037:GLY:HA3	1:D:2045:ARG:HD3	1.73	0.69
1:B:2093:GLY:HA2	1:B:2228:ARG:HG2	1.74	0.69
1:C:1948:LEU:HD22	1:C:1980:ILE:HD13	1.74	0.69
1:D:2096:THR:OG1	1:D:2218:LYS:NZ	2.25	0.69
1:A:2481:VAL:HG21	1:A:2539:HIS:O	1.91	0.69
1:A:1857:GLU:HB3	1:A:1858:LYS:HD3	1.75	0.69
1:D:2084:LEU:HD11	1:D:2242:ILE:HD13	1.75	0.69
1:B:2084:LEU:HD11	1:B:2242:ILE:HD13	1.75	0.69
1:A:2333:GLN:HB3	1:A:2336:LEU:HD12	1.75	0.69
1:C:2217:GLU:HG3	1:C:2229:ILE:HD11	1.75	0.69
1:A:2242:ILE:HD11	1:A:2482:LYS:HE2	1.75	0.68
3:K:10:DA:H2''	3:K:11:DC:H5'	1.75	0.68
1:A:2427:MET:HG3	1:A:2469:ILE:HD11	1.74	0.68
1:B:2536:LEU:HD22	1:B:2543:LEU:HD12	1.76	0.68
1:C:1963:VAL:HG12	1:C:1987:GLU:HB2	1.75	0.68
3:E:14:DC:H2''	3:E:15:DC:H5''	1.76	0.68
1:D:2383:LYS:NZ	6:D:2604:DDS:O3G	2.18	0.67
2:H:4:DG:H2''	2:H:5:DC:H5''	1.76	0.67
1:A:1965:TYR:HB3	1:A:2029:ILE:HG22	1.77	0.67
1:A:2535:ILE:HD11	1:A:2545:GLU:HB3	1.75	0.67
1:C:2333:GLN:HB3	1:C:2336:LEU:HD12	1.76	0.67
1:A:1897:ASP:O	1:A:1977:SER:OG	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1941:LEU:HD23	1:C:1944:ARG:HH12	1.59	0.67
1:D:1963:VAL:HG11	1:D:2057:MET:HG2	1.77	0.67
1:C:2568:LEU:HD12	1:C:2570:VAL:H	1.59	0.67
1:D:2179:THR:OG1	2:L:9:DC:O5'	2.10	0.67
1:A:1940:THR:O	1:A:1944:ARG:NH1	2.27	0.67
1:B:2030:GLN:HB3	1:B:2045:ARG:HB3	1.75	0.67
1:C:2030:GLN:O	1:C:2045:ARG:NH1	2.28	0.67
1:C:2117:ALA:HA	1:C:2193:LEU:HD21	1.77	0.67
1:B:1963:VAL:HG11	1:B:2057:MET:HG2	1.77	0.67
1:A:2037:GLY:O	1:A:2041:SER:N	2.28	0.66
1:D:1972:LYS:HG2	1:D:2089:LEU:HD21	1.77	0.66
3:K:4:DT:H2'	3:K:5:DG:C8	2.29	0.66
1:A:2321:PHE:HB2	1:A:2322:PRO:HD2	1.78	0.66
1:D:2038:SER:HA	1:D:2041:SER:HB2	1.76	0.66
1:C:2077:GLU:OE2	1:C:2482:LYS:NZ	2.28	0.66
1:D:1902:GLY:HA2	1:D:1917:LEU:HD13	1.77	0.66
1:D:2030:GLN:O	1:D:2045:ARG:NH1	2.29	0.66
3:G:5:DG:H2'	3:G:6:DA:C8	2.30	0.66
1:C:2041:SER:HA	1:C:2045:ARG:HE	1.61	0.65
1:B:1897:ASP:O	1:B:1977:SER:OG	2.15	0.65
1:B:2577:LYS:HA	1:B:2586:LYS:HB2	1.78	0.65
1:A:2096:THR:OG1	1:A:2218:LYS:NZ	2.29	0.65
1:D:2201:ARG:HH12	2:L:9:DC:H4'	1.62	0.65
1:B:2077:GLU:OE2	1:B:2482:LYS:NZ	2.30	0.65
1:B:2096:THR:OG1	1:B:2218:LYS:NZ	2.27	0.65
6:B:2604:DDS:C8	2:H:13:DC:H2'	2.27	0.65
1:A:1956:SER:O	1:A:1958:LYS:N	2.30	0.65
1:A:1948:LEU:HD22	1:A:1980:ILE:HD13	1.78	0.64
1:D:2380:GLN:HE22	1:D:2383:LYS:HD2	1.62	0.64
2:H:1:DG:H1	3:G:17:DC:H42	1.43	0.64
2:L:4:DG:H2''	2:L:5:DC:H5''	1.78	0.64
1:B:2383:LYS:NZ	6:B:2604:DDS:O2G	2.30	0.64
1:D:2209:LYS:HE3	3:K:9:DG:H21	1.63	0.64
1:A:2217:GLU:HG3	1:A:2229:ILE:HD11	1.78	0.64
1:B:2190:LEU:HG	1:B:2192:PRO:HD2	1.79	0.64
1:B:2499:PHE:HZ	1:B:2505:ARG:NE	1.95	0.64
1:B:2333:GLN:HB3	1:B:2336:LEU:HD12	1.80	0.64
1:B:1940:THR:O	1:B:1944:ARG:NH1	2.31	0.64
1:B:2220:LEU:HA	1:B:2227:GLU:HA	1.79	0.64
1:D:2337:ARG:HG2	1:D:2352:LEU:HD21	1.80	0.64
1:B:1972:LYS:HG2	1:B:2089:LEU:HD21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2217:GLU:OE1	1:A:2246:GLU:HB3	1.98	0.63
1:A:2568:LEU:HD12	1:A:2570:VAL:H	1.62	0.63
1:A:2241:ARG:HD3	1:A:2539:HIS:CE1	2.33	0.63
6:D:2604:DDS:H8	2:L:13:DC:H2'	1.81	0.63
1:B:2374:VAL:HG13	1:B:2378:LEU:HD23	1.80	0.63
1:A:1834:GLN:HG2	1:A:1939:LEU:HD13	1.81	0.63
1:D:2577:LYS:HA	1:D:2586:LYS:HB2	1.81	0.63
1:B:1994:TRP:CD1	1:B:2236:HIS:HA	2.34	0.62
1:B:2087:LEU:HB2	1:B:2534:PHE:CD2	2.34	0.62
1:D:2190:LEU:HG	1:D:2192:PRO:HD2	1.81	0.62
1:C:2241:ARG:HD3	1:C:2539:HIS:CE1	2.35	0.62
2:H:10:DA:H2'	2:H:11:DT:H5'	1.80	0.62
1:B:2217:GLU:HG3	1:B:2229:ILE:HD11	1.82	0.62
1:C:2374:VAL:HG13	1:C:2378:LEU:HD23	1.82	0.62
1:C:2037:GLY:O	1:C:2041:SER:N	2.33	0.62
1:B:2321:PHE:HB2	1:B:2322:PRO:HD2	1.82	0.62
1:C:2252:VAL:O	1:C:2315:ARG:NH2	2.33	0.62
2:F:10:DA:H2'	2:F:11:DT:H5'	1.81	0.62
1:D:1948:LEU:HD22	1:D:1980:ILE:HD13	1.82	0.62
1:A:2114:GLU:HA	1:A:2127:PHE:HZ	1.64	0.62
1:D:2041:SER:HA	1:D:2045:ARG:HE	1.65	0.61
1:C:2093:GLY:HA2	1:C:2228:ARG:HG2	1.82	0.61
1:A:1994:TRP:CD1	1:A:2236:HIS:HA	2.36	0.61
1:B:1901:VAL:HG23	1:B:1902:GLY:H	1.64	0.61
1:B:1963:VAL:HG12	1:B:1987:GLU:HB2	1.81	0.61
1:B:2037:GLY:HA3	1:B:2045:ARG:HD3	1.82	0.61
1:B:2242:ILE:HD11	1:B:2482:LYS:HE2	1.81	0.61
1:B:2252:VAL:O	1:B:2315:ARG:NH2	2.34	0.61
1:C:2027:GLN:HG3	1:C:2028:GLY:H	1.66	0.61
1:C:2248:ASN:HD22	3:I:8:DT:H4'	1.66	0.61
1:B:1956:SER:O	1:B:1958:LYS:N	2.34	0.61
1:B:1965:TYR:HB3	1:B:2029:ILE:HG22	1.83	0.61
1:C:2216:ARG:HH21	1:C:2217:GLU:HB3	1.66	0.61
1:D:2201:ARG:NH2	2:L:9:DC:O3'	2.34	0.61
1:A:2536:LEU:HD22	1:A:2543:LEU:HD12	1.83	0.61
1:B:2208:THR:HG23	1:B:2209:LYS:HG3	1.82	0.61
1:D:1857:GLU:HB3	1:D:1858:LYS:HD3	1.83	0.61
1:C:2528:PRO:HD3	1:D:2528:PRO:HD3	1.82	0.61
1:D:2239:THR:HG23	3:K:6:DA:H4'	1.83	0.61
1:B:2117:ALA:HA	1:B:2193:LEU:HD21	1.82	0.60
3:E:13:DG:H2''	3:E:14:DC:H5'	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2209:LYS:HG2	3:K:10:DA:H5"	1.82	0.60
1:A:2350:GLN:O	1:A:2354:THR:HG22	2.01	0.60
1:B:2202:ARG:NH2	2:H:11:DT:OP1	2.35	0.60
1:D:1901:VAL:HG23	1:D:1902:GLY:H	1.67	0.60
3:G:5:DG:H2'	3:G:6:DA:H8	1.67	0.60
3:I:12:DA:H2"	3:I:13:DG:C8	2.37	0.60
1:B:2577:LYS:HG2	1:B:2586:LYS:HB2	1.84	0.60
1:C:2201:ARG:NH2	2:J:9:DC:O3'	2.35	0.60
1:C:2216:ARG:NH2	1:C:2217:GLU:HB3	2.17	0.60
6:D:2604:DDS:C8	2:L:13:DC:H2'	2.32	0.60
1:B:2041:SER:OG	1:B:2045:ARG:NH2	2.31	0.59
1:D:2209:LYS:NZ	3:K:9:DG:N3	2.36	0.59
3:E:15:DC:H2"	3:E:16:DG:H5'	1.84	0.59
3:G:10:DA:H2"	3:G:11:DC:H5'	1.83	0.59
2:H:7:DG:H1	3:G:11:DC:H42	1.48	0.59
1:B:2208:THR:OG1	3:G:11:DC:OP1	2.14	0.59
2:J:2:DC:H4'	2:J:3:DG:OP1	2.01	0.59
1:B:2372:GLU:HG3	1:B:2373:SER:H	1.66	0.59
1:D:1941:LEU:O	1:D:1944:ARG:NH2	2.35	0.59
1:B:2535:ILE:HD11	1:B:2545:GLU:HB3	1.83	0.59
1:C:2187:LEU:HA	1:C:2194:PRO:CG	2.32	0.59
1:D:2427:MET:HG3	1:D:2469:ILE:HD11	1.84	0.59
5:A:2603:CA:CA	6:A:2604:DDS:O1G	1.79	0.59
1:A:1940:THR:HB	1:A:1943:ASP:HB2	1.84	0.59
6:B:2604:DDS:H8	2:H:13:DC:H2'	1.84	0.59
1:C:1844:TRP:CZ3	1:C:1951:CYS:HB3	2.38	0.59
1:C:1857:GLU:HB3	1:C:1858:LYS:HD3	1.84	0.59
1:D:2535:ILE:HD11	1:D:2545:GLU:HB3	1.84	0.59
1:B:1954:LYS:H	1:B:1984:GLN:HE21	1.51	0.59
1:A:2470:ASN:ND2	3:E:5:DG:H2"	2.18	0.59
2:L:13:DC:H42	3:K:5:DG:H1	1.50	0.59
1:C:2470:ASN:ND2	3:I:5:DG:H2"	2.18	0.58
2:L:9:DC:N4	3:K:9:DG:H1	1.99	0.58
1:D:2130:SER:HA	1:D:2133:ILE:HD12	1.84	0.58
1:A:2041:SER:HA	1:A:2045:ARG:HE	1.69	0.58
1:B:1844:TRP:CZ3	1:B:1951:CYS:HB3	2.38	0.58
1:B:2193:LEU:HG	1:B:2196:LEU:HD13	1.84	0.58
1:C:2350:GLN:O	1:C:2354:THR:HG22	2.03	0.58
2:H:8:DT:C2'	2:H:9:DC:H5"	2.33	0.58
1:B:1941:LEU:HD23	1:B:1944:ARG:HH12	1.68	0.58
1:A:2102:GLN:NE2	1:A:2313:SER:O	2.25	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1956:SER:O	1:D:1958:LYS:N	2.36	0.58
3:I:5:DG:H2'	3:I:6:DA:H8	1.68	0.58
1:D:2350:GLN:O	1:D:2354:THR:HG22	2.04	0.58
1:A:1902:GLY:HA2	1:A:1917:LEU:HD13	1.85	0.58
1:C:2087:LEU:HD12	1:C:2534:PHE:CE2	2.38	0.58
1:C:2481:VAL:HG21	1:C:2539:HIS:O	2.03	0.58
1:A:1968:ILE:HD13	1:A:2233:SER:HB3	1.86	0.57
1:B:2500:LYS:HD2	1:B:2504:HIS:CE1	2.38	0.57
1:C:2030:GLN:HB3	1:C:2045:ARG:HB3	1.86	0.57
1:A:2190:LEU:HG	1:A:2192:PRO:HD2	1.85	0.57
1:B:1834:GLN:HG2	1:B:1939:LEU:HD13	1.86	0.57
1:C:2072:VAL:O	1:C:2076:VAL:HB	2.04	0.57
2:J:11:DT:H5'	2:J:11:DT:H6	1.69	0.57
1:C:2096:THR:OG1	1:C:2218:LYS:NZ	2.36	0.57
1:A:2459:TYR:HA	3:E:3:DT:H72	1.86	0.57
2:L:5:DC:H42	3:K:13:DG:H1	1.52	0.57
1:D:1844:TRP:CZ3	1:D:1951:CYS:HB3	2.38	0.57
1:D:2220:LEU:HA	1:D:2227:GLU:HA	1.86	0.57
2:H:10:DA:C2'	2:H:11:DT:H5'	2.35	0.57
3:I:5:DG:H2''	3:I:6:DA:H5'	1.85	0.57
1:B:2467:GLN:NE2	3:G:6:DA:OP1	2.37	0.57
1:D:2074:ARG:HG3	1:D:2075:LYS:HG2	1.85	0.57
1:A:2577:LYS:HG2	1:A:2586:LYS:HB2	1.86	0.57
1:B:2387:TYR:HA	1:B:2390:ILE:HD12	1.86	0.57
1:C:2337:ARG:NH1	1:C:2571:LYS:O	2.38	0.57
1:C:1897:ASP:O	1:C:1977:SER:OG	2.23	0.57
1:C:2190:LEU:HG	1:C:2192:PRO:HD2	1.87	0.57
2:F:8:DT:H2''	2:F:9:DC:H5'	1.85	0.57
1:A:2102:GLN:HA	1:A:2105:ILE:HD12	1.85	0.57
1:A:1901:VAL:HG23	1:A:1902:GLY:H	1.70	0.57
1:D:2102:GLN:HA	1:D:2105:ILE:HD12	1.85	0.57
2:H:6:DT:H2''	2:H:7:DG:O4'	2.04	0.57
1:D:2135:GLU:O	1:D:2139:LEU:HB2	2.05	0.57
1:B:2064:LEU:HD23	1:B:2073:PHE:HB2	1.86	0.56
1:D:1969:GLN:HA	1:D:1972:LYS:HE3	1.87	0.56
1:B:1956:SER:C	1:B:1958:LYS:H	2.09	0.56
1:C:2321:PHE:HB2	1:C:2322:PRO:HD2	1.85	0.56
1:D:2027:GLN:HG3	1:D:2028:GLY:H	1.70	0.56
1:B:2029:ILE:HG13	1:B:2031:SER:H	1.68	0.56
1:B:2241:ARG:HD3	1:B:2539:HIS:CE1	2.40	0.56
1:C:2366:TRP:CD1	1:C:2367:LYS:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2193:LEU:HG	1:C:2196:LEU:HD13	1.87	0.56
1:C:1901:VAL:HG23	1:C:1902:GLY:H	1.70	0.56
1:A:1941:LEU:HD23	1:A:1944:ARG:HH12	1.71	0.56
1:C:1940:THR:O	1:C:1944:ARG:NH1	2.39	0.56
1:D:2446:ARG:NH1	1:D:2479:ASP:OD1	2.37	0.56
1:C:2577:LYS:HG2	1:C:2586:LYS:HB2	1.88	0.56
1:D:1834:GLN:HG2	1:D:1939:LEU:HD13	1.87	0.56
1:B:2364:ALA:O	1:B:2369:ILE:HA	2.06	0.56
1:C:1964:ILE:O	1:C:1989:PRO:HD2	2.06	0.56
1:D:2120:LEU:HD12	1:D:2193:LEU:HD22	1.86	0.56
3:E:4:DT:H2'	3:E:5:DG:C8	2.40	0.56
1:B:2350:GLN:O	1:B:2354:THR:HG22	2.06	0.56
1:B:2576:VAL:O	1:B:2586:LYS:HG3	2.06	0.56
1:C:2535:ILE:HD11	1:C:2545:GLU:HB3	1.88	0.56
1:D:1852:ILE:HG12	1:D:1905:VAL:HG22	1.87	0.56
1:C:1834:GLN:HG2	1:C:1939:LEU:HD13	1.88	0.55
1:D:2193:LEU:HG	1:D:2196:LEU:HD13	1.88	0.55
1:D:2321:PHE:HB2	1:D:2322:PRO:HD2	1.88	0.55
1:B:2337:ARG:HG2	1:B:2352:LEU:CD2	2.36	0.55
1:D:2243:THR:HA	1:D:2250:GLN:HE22	1.70	0.55
1:B:2368:MET:HG2	1:D:2421:THR:OG1	2.05	0.55
1:C:2176:GLN:NE2	2:J:8:DT:OP1	2.39	0.55
1:B:2399:GLY:O	1:B:2404:ILE:N	2.40	0.55
1:A:1963:VAL:HG11	1:A:2057:MET:HG2	1.88	0.55
1:A:2241:ARG:HD3	1:A:2539:HIS:ND1	2.22	0.55
1:A:2534:PHE:HA	1:A:2544:TYR:CD1	2.42	0.55
1:A:2335:GLU:CD	6:A:2604:DDS:H2'A	2.27	0.55
1:A:2125:PHE:CZ	1:A:2136:VAL:HB	2.42	0.55
1:D:1960:CYS:SG	1:D:1984:GLN:NE2	2.80	0.55
1:C:1972:LYS:HG2	1:C:2089:LEU:HD21	1.88	0.55
1:C:2372:GLU:HG3	1:C:2373:SER:H	1.72	0.55
1:A:2038:SER:HA	1:A:2041:SER:HB2	1.88	0.54
1:A:2102:GLN:HG2	1:A:2105:ILE:HD12	1.89	0.54
1:A:2372:GLU:HG3	1:A:2373:SER:H	1.71	0.54
2:H:1:DG:H1	3:G:17:DC:N4	2.04	0.54
3:K:5:DG:H2'	3:K:6:DA:H8	1.72	0.54
1:A:2041:SER:OG	1:A:2045:ARG:NH2	2.34	0.54
1:D:1941:LEU:HD23	1:D:1944:ARG:HH12	1.71	0.54
1:D:1963:VAL:HG12	1:D:1987:GLU:HB2	1.90	0.54
1:D:2372:GLU:HG3	1:D:2373:SER:H	1.71	0.54
3:K:10:DA:C2'	3:K:11:DC:H5'	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1964:ILE:O	1:A:1989:PRO:HD2	2.08	0.54
1:A:2014:PRO:HA	1:A:2017:LEU:HD23	1.88	0.54
1:B:1952:LEU:HD23	1:B:1982:LEU:HD13	1.87	0.54
1:A:1956:SER:C	1:A:1958:LYS:H	2.11	0.54
1:D:2364:ALA:O	1:D:2369:ILE:HA	2.08	0.54
1:B:2540:ASP:CG	6:B:2604:DDS:H5'	2.27	0.54
1:C:2201:ARG:HH22	2:J:9:DC:H4'	1.71	0.54
1:C:2568:LEU:HD11	1:C:2572:LEU:HD21	1.90	0.54
1:A:2205:ASN:HD22	2:F:11:DT:H5''	1.73	0.54
1:C:2029:ILE:HG13	1:C:2031:SER:H	1.73	0.54
1:D:2481:VAL:HG21	1:D:2539:HIS:O	2.08	0.54
3:G:16:DG:H2''	3:G:17:DC:C5	2.43	0.54
1:A:2109:LYS:HG2	1:A:2258:ILE:HD11	1.88	0.54
1:C:1852:ILE:HG12	1:C:1905:VAL:HG22	1.90	0.54
1:C:2245:THR:HA	1:C:2247:PRO:O	2.08	0.54
1:C:1960:CYS:SG	1:C:1984:GLN:NE2	2.81	0.53
1:D:2387:TYR:CE1	6:D:2604:DDS:H2'	2.43	0.53
1:A:1844:TRP:CZ3	1:A:1951:CYS:HB3	2.43	0.53
1:A:2027:GLN:HG3	1:A:2028:GLY:H	1.73	0.53
1:C:2205:ASN:ND2	2:J:11:DT:H5''	2.23	0.53
1:A:2100:GLU:HG3	1:A:2103:LYS:HD2	1.90	0.53
1:C:2427:MET:HG3	1:C:2469:ILE:HD11	1.91	0.53
1:A:2029:ILE:HG13	1:A:2031:SER:H	1.74	0.53
1:A:2030:GLN:O	1:A:2045:ARG:NH1	2.40	0.53
1:A:2463:HIS:HA	1:A:2466:ARG:NH1	2.24	0.53
1:A:2488:ILE:HD13	1:A:2558:VAL:HG22	1.90	0.53
1:B:1964:ILE:O	1:B:1989:PRO:HD2	2.08	0.53
1:A:1837:PHE:O	1:A:1840:PHE:HB3	2.08	0.53
1:A:2114:GLU:HA	1:A:2127:PHE:CZ	2.42	0.53
1:A:2205:ASN:OD1	1:A:2209:LYS:HD2	2.08	0.53
1:B:1857:GLU:HB3	1:B:1858:LYS:HD3	1.89	0.53
1:B:2366:TRP:CD1	1:B:2367:LYS:HG3	2.44	0.53
1:D:2041:SER:OG	1:D:2045:ARG:NH2	2.31	0.53
1:A:2100:GLU:O	1:A:2103:LYS:HB3	2.09	0.53
1:A:2135:GLU:O	1:A:2139:LEU:HB2	2.09	0.53
1:C:2077:GLU:O	1:C:2080:SER:HB3	2.09	0.53
1:C:2187:LEU:HD12	1:C:2195:GLY:HA2	1.90	0.53
1:D:2093:GLY:HA2	1:D:2228:ARG:HG2	1.91	0.53
3:K:12:DA:H2''	3:K:13:DG:C8	2.43	0.53
1:C:1994:TRP:CD1	1:C:2236:HIS:HA	2.44	0.53
1:C:1834:GLN:HG3	1:D:1838:GLN:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2243:THR:HA	1:D:2250:GLN:NE2	2.23	0.53
1:D:2252:VAL:O	1:D:2315:ARG:NH2	2.41	0.53
3:E:5:DG:H2"	3:E:6:DA:H5'	1.90	0.53
3:G:5:DG:H2"	3:G:6:DA:H5'	1.90	0.53
6:B:2604:DDS:O5'	6:B:2604:DDS:H8	2.09	0.53
1:C:1941:LEU:HA	1:C:1944:ARG:NH1	2.24	0.53
1:A:2077:GLU:OE2	1:A:2482:LYS:NZ	2.42	0.53
1:B:1983:GLU:O	1:B:1984:GLN:HG3	2.09	0.53
1:C:1983:GLU:O	1:C:1984:GLN:HG3	2.09	0.53
1:C:2012:PHE:O	1:C:2014:PRO:HD3	2.09	0.53
1:D:2077:GLU:OE2	1:D:2482:LYS:NZ	2.40	0.53
1:D:2532:GLY:HA2	1:D:2546:VAL:HA	1.89	0.53
1:B:2069:LEU:HD21	1:B:2445:GLY:O	2.10	0.52
1:C:2340:ALA:HB1	1:C:2349:ILE:HD13	1.91	0.52
1:B:1940:THR:HB	1:B:1943:ASP:HB2	1.90	0.52
1:B:1941:LEU:O	1:B:1944:ARG:NH2	2.42	0.52
1:C:2532:GLY:HA2	1:C:2546:VAL:HA	1.92	0.52
3:K:9:DG:H2"	3:K:10:DA:H5'	1.91	0.52
1:A:2074:ARG:HG3	1:A:2075:LYS:HG2	1.91	0.52
1:A:2441:GLN:HG3	1:A:2447:ARG:HB3	1.90	0.52
1:C:2205:ASN:OD1	1:C:2209:LYS:HD2	2.09	0.52
1:D:2217:GLU:HG3	1:D:2229:ILE:HD11	1.91	0.52
1:A:2499:PHE:HZ	1:A:2505:ARG:NE	1.99	0.52
1:D:2087:LEU:HD12	1:D:2534:PHE:CE2	2.43	0.52
1:A:1952:LEU:HD23	1:A:1982:LEU:HD13	1.90	0.52
1:A:2391:TYR:CE1	1:A:2473:VAL:HG11	2.45	0.52
1:B:1954:LYS:H	1:B:1984:GLN:NE2	2.08	0.52
1:B:2498:THR:OG1	1:B:2499:PHE:N	2.41	0.52
1:D:2576:VAL:O	1:D:2586:LYS:HG3	2.09	0.52
1:D:2040:HIS:HB3	1:D:2044:TYR:CD2	2.45	0.52
1:D:2089:LEU:O	1:D:2230:TYR:HE2	1.93	0.52
1:A:2205:ASN:ND2	2:F:11:DT:H5"	2.24	0.52
1:A:2012:PHE:O	1:A:2014:PRO:HD3	2.10	0.52
1:A:2577:LYS:HA	1:A:2586:LYS:HB2	1.91	0.52
1:B:2470:ASN:ND2	3:G:5:DG:H2"	2.25	0.52
1:C:2038:SER:HA	1:C:2041:SER:HB2	1.92	0.52
1:D:1940:THR:O	1:D:1944:ARG:NH1	2.43	0.52
2:F:10:DA:C2'	2:F:11:DT:H5'	2.39	0.52
1:D:2349:ILE:HD12	1:D:2570:VAL:HG13	1.93	0.51
3:I:4:DT:H2'	3:I:5:DG:H8	1.72	0.51
1:C:2209:LYS:NZ	3:I:9:DG:N3	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1973:ILE:HG23	1:C:1977:SER:HB2	1.92	0.51
1:C:2448:ARG:NH1	1:C:2471:THR:OG1	2.40	0.51
1:C:1956:SER:O	1:C:1958:LYS:N	2.44	0.51
1:C:2463:HIS:O	1:C:2467:GLN:HB2	2.10	0.51
1:D:1983:GLU:O	1:D:1984:GLN:HG3	2.10	0.51
1:D:2380:GLN:NE2	1:D:2383:LYS:HD2	2.26	0.51
1:D:2534:PHE:HA	1:D:2544:TYR:HD1	1.76	0.51
1:A:1849:ARG:HG2	1:A:2054:PHE:CE1	2.44	0.51
1:C:2217:GLU:OE1	1:C:2246:GLU:HB3	2.10	0.51
1:D:1848:LYS:O	1:D:1960:CYS:HB2	2.11	0.51
1:A:2391:TYR:HE1	1:A:2473:VAL:HG11	1.75	0.51
2:L:6:DT:H2''	2:L:7:DG:O4'	2.11	0.51
1:A:2482:LYS:O	1:A:2485:THR:OG1	2.20	0.51
1:B:2241:ARG:HD3	1:B:2539:HIS:ND1	2.26	0.51
1:C:1941:LEU:O	1:C:1944:ARG:NH2	2.44	0.51
1:A:2498:THR:OG1	1:A:2499:PHE:N	2.41	0.50
1:B:1969:GLN:HA	1:B:1972:LYS:HE3	1.94	0.50
1:B:2135:GLU:O	1:B:2139:LEU:HB2	2.12	0.50
1:B:2481:VAL:HG21	1:B:2539:HIS:O	2.11	0.50
1:C:1954:LYS:H	1:C:1984:GLN:HE21	1.57	0.50
1:D:1837:PHE:O	1:D:1840:PHE:HB3	2.11	0.50
1:D:1941:LEU:HA	1:D:1944:ARG:NH1	2.26	0.50
1:D:1991:VAL:HG21	1:D:2081:GLN:HG3	1.93	0.50
1:A:2249:ILE:HA	1:A:2252:VAL:HG13	1.93	0.50
1:C:2360:ARG:HB3	1:C:2372:GLU:OE1	2.11	0.50
2:H:5:DC:N3	3:G:13:DG:N2	2.46	0.50
1:B:1849:ARG:HG2	1:B:2054:PHE:CE1	2.47	0.50
1:C:1902:GLY:HA2	1:C:1917:LEU:HD13	1.93	0.50
1:D:2030:GLN:HB3	1:D:2045:ARG:HB3	1.93	0.50
1:A:2399:GLY:O	1:A:2404:ILE:N	2.43	0.50
6:C:2604:DDS:O1B	6:C:2604:DDS:O1A	2.27	0.50
1:D:2117:ALA:HA	1:D:2193:LEU:HD21	1.92	0.50
1:D:2094:PHE:HZ	1:D:2099:CYS:HB2	1.77	0.50
1:A:2463:HIS:O	1:A:2467:GLN:HB2	2.11	0.50
1:C:1954:LYS:H	1:C:1984:GLN:NE2	2.10	0.50
1:C:2074:ARG:HG3	1:C:2075:LYS:HG2	1.93	0.50
1:B:2202:ARG:NH1	2:H:12:DT:OP1	2.45	0.50
2:L:2:DC:H2''	2:L:3:DG:O5'	2.10	0.50
1:D:2012:PHE:O	1:D:2014:PRO:HD3	2.12	0.50
1:D:2536:LEU:HD22	1:D:2543:LEU:HD12	1.94	0.50
1:D:1968:ILE:HD13	1:D:2233:SER:HB3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1990:LYS:HB2	1:D:2003:PRO:HG2	1.94	0.50
1:B:1843:GLU:O	1:B:1846:CYS:HB3	2.12	0.50
1:C:1972:LYS:O	1:C:1976:LEU:HB2	2.12	0.50
1:C:2207:ILE:HA	1:C:2211:VAL:HG23	1.92	0.50
1:C:2041:SER:OG	1:C:2045:ARG:NH2	2.36	0.49
1:C:2242:ILE:HD11	1:C:2482:LYS:HE2	1.94	0.49
1:A:2238:ALA:HB1	1:A:2448:ARG:CZ	2.43	0.49
1:B:2022:GLY:O	1:B:2040:HIS:NE2	2.44	0.49
1:C:2354:THR:HG23	1:C:2355:GLY:N	2.26	0.49
1:C:2433:ASN:O	1:C:2436:ARG:HG2	2.12	0.49
1:D:2534:PHE:HA	1:D:2544:TYR:CD1	2.47	0.49
1:B:2074:ARG:HG3	1:B:2075:LYS:HG2	1.93	0.49
1:C:1983:GLU:HA	1:C:1986:TYR:OH	2.12	0.49
1:A:1994:TRP:NE1	1:A:2236:HIS:HA	2.28	0.49
1:D:2340:ALA:HB1	1:D:2349:ILE:HD13	1.94	0.49
2:F:8:DT:C2'	2:F:9:DC:H5'	2.43	0.49
1:B:2239:THR:HG23	3:G:6:DA:H4'	1.93	0.49
1:A:1852:ILE:HG12	1:A:1905:VAL:HG22	1.94	0.49
1:A:2342:LEU:HB3	1:A:2426:PHE:CE1	2.48	0.49
1:B:1825:LEU:HD11	1:B:1827:ILE:HG12	1.95	0.49
1:B:2012:PHE:O	1:B:2014:PRO:HD3	2.13	0.49
1:B:2209:LYS:HE3	3:G:9:DG:H21	1.77	0.49
1:C:2424:ASN:HD22	1:C:2424:ASN:C	2.16	0.49
1:A:2538:LEU:HB2	1:A:2541:GLU:CB	2.43	0.49
1:B:2087:LEU:O	1:B:2090:ASN:N	2.46	0.49
3:K:12:DA:H2''	3:K:13:DG:H8	1.78	0.49
1:A:1965:TYR:HE2	1:A:2028:GLY:HA2	1.77	0.49
1:B:2204:THR:O	1:B:2208:THR:HG22	2.13	0.49
1:B:2482:LYS:O	1:B:2485:THR:OG1	2.23	0.49
1:D:1952:LEU:HD23	1:D:1982:LEU:HD13	1.93	0.49
1:A:1859:ILE:O	1:A:1859:ILE:HG23	2.13	0.49
1:A:2030:GLN:HB3	1:A:2045:ARG:HB3	1.94	0.49
1:A:2187:LEU:HD11	1:A:2198:LEU:HD22	1.95	0.49
1:C:2232:VAL:O	1:C:2244:PHE:HA	2.12	0.49
2:J:6:DT:H2''	2:J:7:DG:C8	2.47	0.49
1:D:2179:THR:HG23	2:L:9:DC:OP1	2.13	0.49
1:A:2127:PHE:HB2	1:A:2200:TRP:CH2	2.48	0.49
1:B:1941:LEU:HA	1:B:1944:ARG:NH1	2.28	0.49
1:B:2420:TYR:HB2	1:B:2423:ILE:HD12	1.95	0.49
1:B:2256:PHE:CZ	1:B:2312:ILE:HD11	2.48	0.48
1:C:2397:SER:O	1:C:2400:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2463:HIS:O	1:D:2467:GLN:HB2	2.13	0.48
1:D:2498:THR:OG1	1:D:2499:PHE:N	2.46	0.48
1:D:2568:LEU:HD12	1:D:2570:VAL:H	1.78	0.48
1:B:2427:MET:HG3	1:B:2469:ILE:CD1	2.39	0.48
3:G:1:DC:H2''	3:G:2:DG:C8	2.48	0.48
1:A:1983:GLU:O	1:A:1984:GLN:HG3	2.13	0.48
1:B:2546:VAL:HG21	1:B:2554:VAL:HG21	1.96	0.48
1:C:2499:PHE:HZ	1:C:2505:ARG:NE	2.03	0.48
1:D:1943:ASP:OD1	1:D:1943:ASP:N	2.46	0.48
1:D:2141:LEU:HD13	1:D:2186:LYS:HZ1	1.78	0.48
1:D:2391:TYR:HE1	1:D:2473:VAL:HG11	1.77	0.48
1:A:2415:SER:O	1:A:2419:ARG:HG2	2.13	0.48
1:B:2354:THR:HG23	1:B:2355:GLY:N	2.28	0.48
2:J:7:DG:H1	3:I:11:DC:H42	1.62	0.48
1:A:2100:GLU:HA	1:A:2103:LYS:HE3	1.95	0.48
1:C:2014:PRO:HA	1:C:2017:LEU:HD23	1.95	0.48
1:D:2446:ARG:HH12	1:D:2479:ASP:CG	2.16	0.48
3:E:5:DG:H2'	3:E:6:DA:H8	1.75	0.48
1:B:2359:PHE:CE1	1:B:2383:LYS:HG3	2.49	0.48
1:C:1837:PHE:O	1:C:1840:PHE:HB3	2.13	0.48
1:C:2047:SER:O	1:C:2051:ILE:HG22	2.12	0.48
1:A:2117:ALA:HA	1:A:2193:LEU:HD21	1.94	0.48
1:A:2335:GLU:OE1	1:A:2391:TYR:OH	2.31	0.48
1:B:2090:ASN:OD1	1:B:2501:SER:HB2	2.14	0.48
2:L:12:DT:H3	3:K:6:DA:H2	1.58	0.48
1:A:2239:THR:HG23	3:E:6:DA:H4'	1.95	0.48
1:A:2546:VAL:HG21	1:A:2554:VAL:HG21	1.96	0.48
1:B:2065:GLN:HB2	1:B:2070:GLN:OE1	2.14	0.48
1:C:2100:GLU:O	1:C:2103:LYS:HB3	2.14	0.48
1:D:2087:LEU:HB2	1:D:2534:PHE:CD2	2.49	0.48
1:C:2534:PHE:HA	1:C:2544:TYR:HD1	1.79	0.48
1:A:2254:ARG:NH1	2:F:13:DC:OP2	2.46	0.48
2:H:10:DA:H3'	2:H:11:DT:H71	1.95	0.48
2:L:10:DA:C2'	2:L:11:DT:H5'	2.44	0.48
1:A:1941:LEU:O	1:A:1944:ARG:NH2	2.46	0.48
1:A:2125:PHE:HZ	1:A:2136:VAL:HB	1.77	0.48
1:A:2340:ALA:HB1	1:A:2349:ILE:HD13	1.96	0.48
1:B:2241:ARG:HD3	1:B:2539:HIS:CG	2.48	0.48
1:C:2113:ILE:HG23	1:C:2196:LEU:HG	1.96	0.48
1:C:2320:PRO:HG3	1:C:2325:SER:HA	1.96	0.48
1:D:2482:LYS:O	1:D:2485:THR:OG1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:GLN:HA	1:A:1972:LYS:HB2	1.94	0.47
1:B:2038:SER:HA	1:B:2041:SER:HB2	1.95	0.47
1:B:2047:SER:O	1:B:2051:ILE:HG22	2.13	0.47
1:A:2113:ILE:HG23	1:A:2196:LEU:HG	1.96	0.47
1:A:2469:ILE:O	1:A:2473:VAL:HG12	2.13	0.47
1:A:2534:PHE:HA	1:A:2544:TYR:HD1	1.77	0.47
1:C:2364:ALA:O	1:C:2369:ILE:HA	2.14	0.47
1:B:2176:GLN:NE2	2:H:8:DT:OP1	2.46	0.47
2:L:10:DA:H2'	2:L:11:DT:H5'	1.95	0.47
1:A:1941:LEU:HA	1:A:1944:ARG:NH1	2.29	0.47
1:B:2071:ASP:O	1:B:2075:LYS:HB2	2.14	0.47
1:B:2338:ILE:HD11	1:B:2477:ALA:HA	1.95	0.47
1:D:1859:ILE:HG23	1:D:1859:ILE:O	2.14	0.47
1:D:1969:GLN:HA	1:D:1972:LYS:HB2	1.95	0.47
1:D:2335:GLU:CD	6:D:2604:DDS:H2'A	2.34	0.47
3:E:9:DG:C2'	3:E:10:DA:H5''	2.40	0.47
2:L:13:DC:N3	3:K:5:DG:N2	2.59	0.47
1:B:2347:ARG:O	1:B:2351:VAL:HG23	2.14	0.47
1:C:2383:LYS:HD3	6:C:2604:DDS:O3A	2.13	0.47
1:D:2467:GLN:HA	1:D:2470:ASN:OD1	2.14	0.47
3:G:1:DC:O2	3:G:1:DC:H5''	2.14	0.47
2:L:13:DC:N4	3:K:5:DG:H1	2.10	0.47
1:C:2576:VAL:O	1:C:2586:LYS:HG3	2.13	0.47
1:D:2050:SER:OG	1:D:2051:ILE:N	2.48	0.47
1:A:1983:GLU:HA	1:A:1986:TYR:OH	2.13	0.47
1:B:1852:ILE:HG12	1:B:1905:VAL:HG22	1.97	0.47
1:B:2433:ASN:O	1:B:2436:ARG:HG2	2.14	0.47
1:B:2092:ILE:HB	1:B:2535:ILE:HG23	1.96	0.47
1:D:2090:ASN:OD1	1:D:2501:SER:HB2	2.14	0.47
1:D:2354:THR:HG23	1:D:2355:GLY:N	2.30	0.47
1:A:2387:TYR:CE1	6:A:2604:DDS:H2'	2.49	0.47
1:B:2100:GLU:HA	1:B:2103:LYS:HB3	1.97	0.47
1:B:2113:ILE:HG23	1:B:2196:LEU:HG	1.96	0.47
2:J:7:DG:C2'	2:J:8:DT:H5''	2.41	0.47
2:J:8:DT:C2'	2:J:9:DC:H5'	2.37	0.47
1:A:1972:LYS:O	1:A:1976:LEU:HB2	2.15	0.47
1:B:2359:PHE:CZ	1:B:2383:LYS:HG3	2.50	0.47
1:B:2463:HIS:HA	1:B:2466:ARG:NH1	2.30	0.47
3:G:17:DC:H6	3:G:17:DC:H2'	1.55	0.47
1:A:2576:VAL:O	1:A:2586:LYS:HG3	2.15	0.47
1:B:2184:LEU:O	1:B:2187:LEU:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2349:ILE:HD12	1:B:2570:VAL:HG13	1.97	0.47
1:B:2463:HIS:O	1:B:2467:GLN:HB2	2.15	0.47
1:D:2245:THR:HA	1:D:2247:PRO:O	2.15	0.47
1:A:1954:LYS:H	1:A:1984:GLN:HE21	1.63	0.47
1:A:2360:ARG:HB3	1:A:2372:GLU:OE1	2.15	0.47
1:A:2481:VAL:O	1:A:2485:THR:HG23	2.15	0.47
1:B:1968:ILE:HG13	1:B:1969:GLN:N	2.30	0.47
1:C:2474:GLN:HE22	3:I:5:DG:N2	2.12	0.47
1:C:2335:GLU:HG3	6:C:2604:DDS:H3'A	1.97	0.47
1:D:2047:SER:O	1:D:2051:ILE:HG22	2.15	0.47
2:L:6:DT:H2"	2:L:7:DG:C8	2.50	0.47
1:B:1960:CYS:SG	1:B:1984:GLN:NE2	2.87	0.46
1:B:1994:TRP:NE1	1:B:2236:HIS:HA	2.30	0.46
1:A:2110:LEU:HD12	1:A:2200:TRP:NE1	2.31	0.46
1:C:2538:LEU:HD12	1:C:2541:GLU:OE2	2.15	0.46
1:B:1977:SER:O	1:B:2510:GLN:HG2	2.16	0.46
1:C:2135:GLU:O	1:C:2139:LEU:HB2	2.15	0.46
1:D:1969:GLN:HE22	1:D:2032:LEU:HD13	1.80	0.46
1:A:2100:GLU:HA	1:A:2103:LYS:HB3	1.97	0.46
1:A:2546:VAL:HG13	1:A:2551:VAL:HG12	1.98	0.46
1:B:1966:ASP:OD2	4:B:2602:GOL:H32	2.15	0.46
1:D:2481:VAL:O	1:D:2485:THR:HG23	2.16	0.46
1:A:1973:ILE:HG23	1:A:1977:SER:HB2	1.98	0.46
1:A:2256:PHE:CZ	1:A:2312:ILE:HD11	2.50	0.46
1:B:2037:GLY:O	1:B:2040:HIS:N	2.49	0.46
1:C:2498:THR:OG1	1:C:2499:PHE:N	2.43	0.46
1:D:2347:ARG:O	1:D:2351:VAL:HG23	2.16	0.46
1:B:2031:SER:HA	1:B:2045:ARG:HH12	1.81	0.46
1:B:2206:ALA:O	1:B:2210:VAL:HB	2.16	0.46
1:D:2038:SER:HA	1:D:2041:SER:CB	2.45	0.46
1:D:2242:ILE:O	1:D:2250:GLN:NE2	2.46	0.46
3:G:9:DG:H2"	3:G:10:DA:H5"	1.98	0.46
1:B:2534:PHE:HA	1:B:2544:TYR:HD1	1.80	0.46
1:C:2533:PHE:N	1:C:2545:GLU:O	2.42	0.46
1:D:2092:ILE:HB	1:D:2535:ILE:HG23	1.98	0.46
1:D:1994:TRP:CD1	1:D:2236:HIS:HA	2.51	0.46
1:B:2221:ASN:HB3	1:B:2224:LEU:HD13	1.97	0.46
1:B:2398:LEU:HD11	1:B:2402:MET:HE3	1.96	0.46
1:B:2443:ILE:HG13	1:B:2476:SER:OG	2.15	0.46
1:B:2047:SER:O	1:B:2050:SER:OG	2.20	0.45
1:B:2087:LEU:HD12	1:B:2534:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2191:HIS:N	1:C:2192:PRO:HD2	2.31	0.45
1:C:2577:LYS:HA	1:C:2586:LYS:HB2	1.98	0.45
1:C:2347:ARG:O	1:C:2351:VAL:HG23	2.16	0.45
3:E:1:DC:H42	3:G:1:DC:N4	2.15	0.45
1:B:2117:ALA:HB2	1:B:2196:LEU:HD21	1.99	0.45
3:K:4:DT:H2'	3:K:5:DG:H8	1.80	0.45
1:B:1837:PHE:O	1:B:1840:PHE:HB3	2.16	0.45
1:C:2059:GLN:O	1:C:2062:SER:HB3	2.16	0.45
1:C:2199:GLU:O	1:C:2203:ILE:HG13	2.16	0.45
1:C:2387:TYR:HA	1:C:2390:ILE:HD12	1.98	0.45
1:B:1990:LYS:HB2	1:B:2003:PRO:HG2	1.99	0.45
1:B:2220:LEU:HD12	1:B:2222:PRO:HD3	1.99	0.45
1:B:2590:VAL:OXT	1:B:2590:VAL:HG22	2.16	0.45
1:C:2113:ILE:HA	1:C:2113:ILE:HD13	1.78	0.45
1:C:2241:ARG:HD3	1:C:2539:HIS:ND1	2.32	0.45
1:D:2221:ASN:HA	1:D:2222:PRO:HD2	1.84	0.45
3:E:1:DC:H3'	3:E:2:DG:H5''	1.98	0.45
2:H:13:DC:H42	3:G:5:DG:H1	1.64	0.45
1:B:2463:HIS:ND1	3:G:5:DG:OP1	2.47	0.45
1:A:2220:LEU:HA	1:A:2227:GLU:HA	1.98	0.45
1:B:2102:GLN:NE2	1:B:2313:SER:O	2.38	0.45
1:D:1956:SER:C	1:D:1958:LYS:H	2.20	0.45
1:A:2199:GLU:O	1:A:2203:ILE:HG13	2.17	0.45
1:B:2100:GLU:HA	1:B:2103:LYS:HE3	1.99	0.45
1:B:2415:SER:O	1:B:2419:ARG:HG2	2.17	0.45
1:B:2534:PHE:HA	1:B:2544:TYR:CD1	2.52	0.45
1:C:1982:LEU:O	1:C:1986:TYR:OH	2.34	0.45
1:C:2037:GLY:HA3	1:C:2045:ARG:HD3	1.97	0.45
1:B:2013:LEU:HG	1:B:2016:GLU:HB2	1.97	0.45
1:C:1952:LEU:HD23	1:C:1982:LEU:HD13	1.98	0.45
1:C:2242:ILE:O	1:C:2250:GLN:NE2	2.45	0.45
1:A:2354:THR:HG23	1:A:2355:GLY:N	2.32	0.45
1:A:2437:ASP:HB3	1:A:2439:PHE:CE1	2.52	0.45
1:A:2446:ARG:HH12	1:A:2479:ASP:CG	2.19	0.45
1:B:1859:ILE:O	1:B:1859:ILE:HG23	2.17	0.45
1:C:1969:GLN:HA	1:C:1972:LYS:HE3	1.98	0.45
1:D:2331:TYR:HB3	1:D:2334:LEU:HB2	1.99	0.45
1:B:1856:CYS:SG	1:B:1900:VAL:HG22	2.56	0.45
1:B:2040:HIS:HB3	1:B:2044:TYR:CD2	2.52	0.45
1:B:2203:ILE:O	1:B:2207:ILE:HG22	2.17	0.45
1:B:1994:TRP:HB2	1:B:2236:HIS:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1849:ARG:HG2	1:C:2054:PHE:CE1	2.51	0.45
1:D:2087:LEU:O	1:D:2090:ASN:N	2.50	0.45
1:D:2543:LEU:HD23	1:D:2543:LEU:HA	1.72	0.45
2:H:7:DG:H1	3:G:11:DC:N4	2.12	0.45
1:A:1856:CYS:SG	1:A:1900:VAL:HG22	2.57	0.44
1:A:2420:TYR:HB2	1:A:2423:ILE:HD12	1.98	0.44
1:C:1956:SER:C	1:C:1958:LYS:H	2.21	0.44
1:D:1838:GLN:O	1:D:1841:ILE:HG13	2.18	0.44
1:C:2090:ASN:ND2	1:C:2534:PHE:O	2.40	0.44
1:D:2206:ALA:O	1:D:2210:VAL:HB	2.17	0.44
1:D:2535:ILE:HD11	1:D:2545:GLU:CB	2.47	0.44
1:D:2584:GLU:C	1:D:2585:LEU:HD12	2.38	0.44
1:A:2089:LEU:O	1:A:2230:TYR:HE2	2.01	0.44
1:A:2106:MET:HE2	1:A:2312:ILE:HD12	1.99	0.44
1:B:2184:LEU:HD12	1:B:2187:LEU:HD22	1.99	0.44
1:B:2205:ASN:OD1	1:B:2209:LYS:HD2	2.17	0.44
1:B:2387:TYR:CE1	6:B:2604:DDS:H2'	2.53	0.44
1:B:2387:TYR:CZ	6:B:2604:DDS:H2'	2.53	0.44
1:B:2404:ILE:HD11	1:B:2409:ALA:HB2	2.00	0.44
1:C:1851:SER:HB3	1:C:1906:CYS:O	2.17	0.44
1:A:2532:GLY:HA2	1:A:2546:VAL:HA	1.98	0.44
1:B:1968:ILE:HD13	1:B:2233:SER:HB3	2.00	0.44
1:B:2346:ARG:HG3	1:B:2347:ARG:N	2.32	0.44
1:B:2380:GLN:HE22	1:B:2383:LYS:HD2	1.82	0.44
1:B:2538:LEU:HB2	1:B:2541:GLU:CB	2.47	0.44
1:C:1859:ILE:O	1:C:1859:ILE:HG23	2.18	0.44
1:C:2405:LYS:HD2	1:C:2405:LYS:N	2.33	0.44
1:C:2542:LEU:HA	1:C:2542:LEU:HD23	1.67	0.44
1:D:2500:LYS:HB2	1:D:2500:LYS:HE2	1.76	0.44
1:B:2248:ASN:HD22	3:G:8:DT:H4'	1.82	0.44
1:D:2209:LYS:HZ2	3:K:9:DG:H1'	1.81	0.44
1:A:2500:LYS:HD2	1:A:2504:HIS:NE2	2.33	0.44
1:C:2191:HIS:O	1:C:2193:LEU:N	2.48	0.44
1:C:2535:ILE:HD11	1:C:2545:GLU:CB	2.47	0.44
1:D:2256:PHE:CZ	1:D:2312:ILE:HD11	2.52	0.44
1:D:2360:ARG:HB3	1:D:2372:GLU:OE1	2.17	0.44
2:L:3:DG:H2''	2:L:4:DG:C8	2.53	0.44
1:D:1852:ILE:HD12	1:D:1962:VAL:HG21	2.00	0.44
1:A:1841:ILE:HD13	1:A:1845:ARG:HE	1.83	0.44
1:A:2087:LEU:HB2	1:A:2534:PHE:CD2	2.52	0.44
1:B:2027:GLN:HG3	1:B:2028:GLY:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2232:VAL:O	1:B:2244:PHE:HA	2.17	0.44
1:C:2412:TYR:O	1:C:2415:SER:HB3	2.18	0.44
1:C:2536:LEU:HD22	1:C:2543:LEU:HD12	1.99	0.44
1:D:2313:SER:HB2	1:D:2316:HIS:HB2	1.99	0.44
1:B:1992:ALA:O	1:B:1996:LEU:HG	2.18	0.44
1:B:2103:LYS:NZ	1:B:2215:GLN:HE22	2.16	0.44
1:C:2469:ILE:O	1:C:2473:VAL:HG12	2.18	0.44
1:C:2087:LEU:HB2	1:C:2534:PHE:CD2	2.53	0.44
1:C:2543:LEU:HA	1:C:2543:LEU:HD23	1.74	0.44
1:D:2079:PRO:HB2	1:D:2486:VAL:HG11	2.00	0.44
1:D:2500:LYS:HD2	1:D:2504:HIS:NE2	2.33	0.44
1:A:2049:GLU:HG2	1:A:2053:ILE:HD12	2.00	0.44
1:C:2031:SER:O	1:C:2034:LEU:HB3	2.17	0.44
1:D:1994:TRP:HB2	1:D:2236:HIS:CE1	2.53	0.44
1:D:2397:SER:O	1:D:2400:GLU:HB3	2.18	0.44
1:A:2470:ASN:OD1	3:E:5:DG:H4'	2.18	0.44
1:B:2077:GLU:O	1:B:2080:SER:HB3	2.18	0.43
1:C:2092:ILE:HG23	1:C:2229:ILE:HG22	2.00	0.43
1:A:2205:ASN:ND2	2:F:10:DA:H2''	2.32	0.43
3:I:10:DA:H2''	3:I:11:DC:C5'	2.48	0.43
1:A:2047:SER:O	1:A:2051:ILE:HG22	2.18	0.43
1:A:2412:TYR:O	1:A:2415:SER:HB3	2.18	0.43
1:C:2534:PHE:HA	1:C:2544:TYR:CD1	2.53	0.43
1:D:2499:PHE:CZ	1:D:2505:ARG:NE	2.78	0.43
1:A:2184:LEU:O	1:A:2187:LEU:N	2.52	0.43
1:A:2583:GLY:C	1:A:2584:GLU:HG3	2.38	0.43
1:B:1841:ILE:HD13	1:B:1845:ARG:HE	1.83	0.43
1:B:2100:GLU:O	1:B:2103:LYS:HB3	2.19	0.43
1:B:2469:ILE:O	1:B:2473:VAL:HG12	2.18	0.43
1:C:2243:THR:HA	1:C:2250:GLN:NE2	2.33	0.43
1:D:2040:HIS:HB3	1:D:2044:TYR:HD2	1.83	0.43
3:G:5:DG:C2'	3:G:6:DA:H5'	2.48	0.43
1:B:2563:GLU:HG2	1:B:2572:LEU:O	2.19	0.43
1:C:2184:LEU:O	1:C:2187:LEU:N	2.48	0.43
1:C:2310:PHE:CG	1:C:2311:SER:N	2.87	0.43
1:D:2071:ASP:O	1:D:2075:LYS:HB2	2.18	0.43
1:D:2391:TYR:CE1	1:D:2473:VAL:HG11	2.52	0.43
1:D:2379:ARG:NH1	6:D:2604:DDS:O2G	2.33	0.43
1:B:2433:ASN:HA	1:B:2436:ARG:HG2	2.00	0.43
1:C:1941:LEU:HA	1:C:1944:ARG:CZ	2.49	0.43
1:C:2481:VAL:O	1:C:2485:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1834:GLN:HG3	1:D:1838:GLN:CB	2.49	0.43
1:A:2466:ARG:NH1	3:E:5:DG:OP1	2.42	0.43
1:A:2008:ILE:HG23	1:A:2012:PHE:CD2	2.54	0.43
1:A:2488:ILE:O	1:A:2492:LEU:HD13	2.19	0.43
1:A:2535:ILE:HD11	1:A:2545:GLU:CB	2.45	0.43
1:B:1899:LEU:HA	1:B:1899:LEU:HD22	1.83	0.43
1:B:2331:TYR:OH	1:B:2562:MET:O	2.25	0.43
1:D:2542:LEU:HA	1:D:2542:LEU:HD23	1.84	0.43
1:A:1903:LEU:HD13	1:A:1948:LEU:HD11	2.01	0.43
1:A:2538:LEU:HD12	1:A:2541:GLU:OE2	2.19	0.43
1:B:1844:TRP:CH2	1:B:1951:CYS:HB3	2.54	0.43
1:C:2220:LEU:HA	1:C:2227:GLU:HA	1.99	0.43
1:D:2094:PHE:CZ	1:D:2099:CYS:HB2	2.54	0.43
1:A:1982:LEU:O	1:A:1986:TYR:OH	2.37	0.43
1:A:2107:GLN:O	1:A:2110:LEU:HB3	2.18	0.43
2:H:7:DG:H4'	2:H:7:DG:OP1	2.18	0.43
2:J:3:DG:H2''	2:J:4:DG:H5''	2.00	0.43
1:A:2499:PHE:CZ	1:A:2505:ARG:NE	2.76	0.43
1:B:1975:LEU:O	1:B:1979:GLY:HA2	2.18	0.43
1:B:2041:SER:CA	1:B:2045:ARG:HE	2.28	0.43
1:B:1972:LYS:HD3	1:B:2088:GLU:OE1	2.19	0.43
1:B:2188:LYS:H	1:B:2188:LYS:HG2	1.71	0.43
1:B:2003:PRO:HD3	1:B:2236:HIS:CE1	2.53	0.43
1:C:1992:ALA:O	1:C:1996:LEU:HG	2.18	0.43
1:C:2391:TYR:HE1	1:C:2473:VAL:HG11	1.84	0.43
1:B:2245:THR:O	1:B:2245:THR:OG1	2.34	0.43
1:C:2221:ASN:HA	1:C:2222:PRO:HD2	1.94	0.43
1:D:2335:GLU:HG2	1:D:2477:ALA:HB2	2.01	0.43
3:E:10:DA:C2'	3:E:11:DC:H5'	2.39	0.43
1:A:2087:LEU:O	1:A:2090:ASN:N	2.52	0.42
1:A:2090:ASN:OD1	1:A:2501:SER:HB2	2.19	0.42
1:B:1982:LEU:O	1:B:1986:TYR:OH	2.36	0.42
1:B:2009:VAL:HG23	1:B:2013:LEU:HB3	2.00	0.42
1:B:2216:ARG:HH21	1:B:2217:GLU:HB3	1.84	0.42
1:B:2543:LEU:HA	1:B:2543:LEU:HD23	1.74	0.42
1:C:1844:TRP:HE1	1:C:1905:VAL:HG11	1.84	0.42
1:C:2184:LEU:O	1:C:2187:LEU:HB3	2.19	0.42
1:D:2444:LEU:HD21	1:D:2483:ILE:HD11	2.01	0.42
2:J:9:DC:H1'	2:J:10:DA:O4'	2.19	0.42
1:A:2141:LEU:HD11	1:A:2190:LEU:CD2	2.49	0.42
1:B:2380:GLN:NE2	1:B:2383:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2546:VAL:HG21	1:D:2554:VAL:HG21	2.02	0.42
1:A:2467:GLN:NE2	3:E:6:DA:OP1	2.52	0.42
2:H:9:DC:H2''	2:H:10:DA:H8	1.84	0.42
1:A:2243:THR:HA	1:A:2250:GLN:NE2	2.34	0.42
1:A:2347:ARG:HH22	1:A:2419:ARG:CZ	2.32	0.42
1:A:2441:GLN:OE1	1:A:2447:ARG:NH2	2.52	0.42
1:C:1965:TYR:HE2	1:C:2028:GLY:HA2	1.83	0.42
3:K:5:DG:H2''	3:K:6:DA:H5'	2.00	0.42
1:A:2364:ALA:O	1:A:2369:ILE:HA	2.19	0.42
1:A:2538:LEU:HB2	1:A:2541:GLU:HB3	2.02	0.42
1:B:2405:LYS:N	1:B:2405:LYS:HD2	2.33	0.42
1:B:2536:LEU:HD23	1:B:2537:GLN:N	2.34	0.42
1:C:2201:ARG:HH22	2:J:9:DC:C4'	2.33	0.42
1:D:2184:LEU:HD12	1:D:2187:LEU:HD22	2.01	0.42
1:D:2505:ARG:HH22	1:D:2529:ILE:HG12	1.84	0.42
3:I:5:DG:C2'	3:I:6:DA:H5'	2.49	0.42
1:A:2349:ILE:HD12	1:A:2570:VAL:HG13	2.02	0.42
1:B:1830:VAL:HG13	1:B:1836:LEU:HD23	2.01	0.42
1:B:2481:VAL:O	1:B:2485:THR:HG23	2.19	0.42
6:B:2604:DDS:H5'A	2:H:13:DC:C2'	2.50	0.42
1:A:1963:VAL:CG1	1:A:1987:GLU:HB2	2.43	0.42
1:A:2340:ALA:HB1	1:A:2349:ILE:CD1	2.49	0.42
1:A:2538:LEU:HB2	1:A:2541:GLU:HB2	2.02	0.42
1:D:1968:ILE:HG22	1:D:2085:ALA:HB2	2.01	0.42
1:A:2333:GLN:O	1:A:2337:ARG:HG3	2.20	0.42
1:A:2500:LYS:HD2	1:A:2504:HIS:CE1	2.55	0.42
1:B:2092:ILE:HA	1:B:2228:ARG:NH2	2.33	0.42
1:B:2103:LYS:HZ3	1:B:2215:GLN:HE22	1.67	0.42
1:C:2102:GLN:HA	1:C:2105:ILE:HD12	2.01	0.42
1:B:2245:THR:HA	1:B:2247:PRO:O	2.20	0.42
1:C:2009:VAL:HG11	1:C:2020:LEU:HD23	2.02	0.42
2:H:2:DC:H4'	2:H:3:DG:OP1	2.19	0.42
1:A:2037:GLY:HA3	1:A:2045:ARG:HD3	2.02	0.42
1:B:2125:PHE:CZ	1:B:2136:VAL:HB	2.55	0.42
1:D:2228:ARG:NH2	1:D:2545:GLU:OE2	2.53	0.42
1:A:2337:ARG:O	1:A:2340:ALA:HB3	2.20	0.42
1:B:2191:HIS:N	1:B:2192:PRO:HD2	2.35	0.42
1:B:2500:LYS:HD2	1:B:2504:HIS:NE2	2.35	0.42
1:C:2446:ARG:HH12	1:C:2479:ASP:CG	2.23	0.42
1:B:2470:ASN:OD1	3:G:5:DG:H4'	2.18	0.42
2:H:3:DG:C6	2:H:4:DG:C6	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:6:DT:C2'	2:L:7:DG:C8	3.03	0.42
1:A:2092:ILE:HA	1:A:2228:ARG:NH2	2.34	0.41
1:B:2349:ILE:HG23	1:B:2570:VAL:CG1	2.50	0.41
1:D:1825:LEU:HD11	1:D:1827:ILE:HG12	2.01	0.41
1:D:2216:ARG:NH2	1:D:2217:GLU:HB3	2.35	0.41
1:B:2050:SER:OG	1:B:2051:ILE:N	2.53	0.41
1:C:1844:TRP:CH2	1:C:1951:CYS:HB3	2.55	0.41
1:D:2412:TYR:O	1:D:2415:SER:HB3	2.20	0.41
1:A:2059:GLN:O	1:A:2062:SER:HB3	2.20	0.41
1:A:2113:ILE:HA	1:A:2113:ILE:HD13	1.81	0.41
1:D:2342:LEU:HB3	1:D:2426:PHE:CE1	2.54	0.41
1:C:2546:VAL:HG21	1:C:2554:VAL:HG21	2.02	0.41
1:D:2059:GLN:O	1:D:2062:SER:HB3	2.21	0.41
1:D:2089:LEU:HA	1:D:2089:LEU:HD23	1.84	0.41
1:D:2129:SER:O	1:D:2133:ILE:HG13	2.21	0.41
1:A:2114:GLU:HG2	1:A:2118:TYR:CE2	2.55	0.41
1:C:1994:TRP:CD1	1:C:1998:PRO:HA	2.55	0.41
1:B:2360:ARG:HB3	1:B:2372:GLU:OE1	2.20	0.41
1:D:2209:LYS:NZ	3:K:10:DA:O4'	2.47	0.41
1:A:2243:THR:HA	1:A:2250:GLN:HE22	1.85	0.41
1:A:2389:ILE:HA	1:A:2393:MET:CB	2.51	0.41
1:C:2087:LEU:O	1:C:2090:ASN:N	2.54	0.41
1:D:2072:VAL:O	1:D:2076:VAL:HB	2.21	0.41
1:D:2424:ASN:HD22	1:D:2424:ASN:C	2.24	0.41
3:G:10:DA:C2'	3:G:11:DC:H5'	2.51	0.41
3:G:14:DC:H6	3:G:14:DC:H2'	1.68	0.41
1:A:2190:LEU:O	1:A:2194:PRO:HG3	2.21	0.41
1:A:2536:LEU:HD23	1:A:2537:GLN:N	2.35	0.41
1:B:2113:ILE:HA	1:B:2113:ILE:HD13	1.84	0.41
1:D:2455:ASP:OD2	1:D:2460:ARG:HD2	2.20	0.41
1:D:2463:HIS:HA	1:D:2466:ARG:NH1	2.36	0.41
1:D:2538:LEU:HD12	1:D:2541:GLU:OE2	2.21	0.41
1:D:2577:LYS:HG2	1:D:2586:LYS:HB2	2.03	0.41
3:E:15:DC:C2'	3:E:16:DG:H5'	2.48	0.41
1:D:2466:ARG:NH1	3:K:5:DG:OP1	2.47	0.41
1:A:1916:SER:C	1:A:1917:LEU:HD12	2.41	0.41
1:A:1969:GLN:O	1:A:1972:LYS:HB2	2.21	0.41
1:A:2366:TRP:CD1	1:A:2367:LYS:HG3	2.55	0.41
1:B:1849:ARG:NH1	1:B:1987:GLU:OE1	2.50	0.41
1:B:2138:PHE:HZ	1:B:2177:PHE:HB2	1.86	0.41
1:C:1941:LEU:O	1:C:1944:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2177:PHE:O	1:D:2178:SER:HB2	2.21	0.41
3:I:10:DA:H2''	3:I:11:DC:H5'	2.02	0.41
1:A:2204:THR:O	1:A:2208:THR:HG22	2.21	0.41
1:B:2205:ASN:CG	2:H:10:DA:H2''	2.41	0.41
1:B:2340:ALA:HB1	1:B:2349:ILE:HD13	2.02	0.41
1:C:1825:LEU:HD11	1:C:1827:ILE:HG12	2.02	0.41
1:C:1855:ALA:HB1	1:C:2045:ARG:HH22	1.86	0.41
1:C:2380:GLN:HE22	1:C:2383:LYS:HD2	1.86	0.41
1:C:2568:LEU:HD21	1:C:2572:LEU:HD21	2.03	0.41
1:D:2092:ILE:HG23	1:D:2229:ILE:HG22	2.02	0.41
1:D:2117:ALA:HB2	1:D:2196:LEU:HD21	2.02	0.41
1:D:2092:ILE:HA	1:D:2228:ARG:NH2	2.36	0.41
2:L:1:DG:N2	2:L:2:DC:O2	2.53	0.41
1:A:2191:HIS:N	1:A:2192:PRO:HD2	2.36	0.41
1:A:2310:PHE:CG	1:A:2311:SER:N	2.89	0.41
1:B:1902:GLY:HA2	1:B:1917:LEU:HD13	2.02	0.41
1:B:1991:VAL:HG21	1:B:2081:GLN:HG3	2.03	0.41
1:B:2424:ASN:HD22	1:B:2424:ASN:C	2.22	0.41
1:B:2538:LEU:HB2	1:B:2541:GLU:HB2	2.03	0.41
1:B:2583:GLY:C	1:B:2584:GLU:HG3	2.41	0.41
1:C:2232:VAL:HG12	1:C:2233:SER:O	2.21	0.41
1:C:2243:THR:HA	1:C:2250:GLN:HE22	1.86	0.41
1:A:1845:ARG:HH11	1:A:1947:TYR:HE1	1.69	0.40
1:B:2059:GLN:O	1:B:2062:SER:HB3	2.21	0.40
1:C:1969:GLN:O	1:C:1972:LYS:HB2	2.22	0.40
1:C:2003:PRO:HD3	1:C:2236:HIS:CE1	2.57	0.40
1:C:2141:LEU:HD11	1:C:2190:LEU:CD2	2.51	0.40
1:C:2536:LEU:HD23	1:C:2537:GLN:N	2.36	0.40
1:D:1969:GLN:O	1:D:1972:LYS:HB2	2.22	0.40
1:D:2241:ARG:HD3	1:D:2539:HIS:CE1	2.56	0.40
3:E:15:DC:H2''	3:E:16:DG:C5'	2.51	0.40
2:J:3:DG:H2''	2:J:4:DG:C8	2.56	0.40
1:A:2546:VAL:CG2	1:A:2554:VAL:HG21	2.51	0.40
1:C:2248:ASN:HD22	3:I:8:DT:C4'	2.33	0.40
1:C:2583:GLY:C	1:C:2584:GLU:HG3	2.41	0.40
1:A:2380:GLN:HE22	1:A:2383:LYS:HD2	1.86	0.40
1:B:2107:GLN:O	1:B:2110:LEU:HB3	2.21	0.40
1:B:2184:LEU:O	1:B:2187:LEU:N	2.54	0.40
1:B:2249:ILE:HA	1:B:2252:VAL:HG13	2.04	0.40
1:B:2310:PHE:CG	1:B:2311:SER:N	2.89	0.40
1:B:2335:GLU:OE2	1:B:2474:GLN:HG2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2090:ASN:ND2	1:C:2533:PHE:HB3	2.36	0.40
1:C:2254:ARG:NH1	2:J:13:DC:OP2	2.54	0.40
1:A:1898:THR:HA	1:A:1977:SER:OG	2.21	0.40
1:B:2217:GLU:OE1	1:B:2246:GLU:HB3	2.22	0.40
1:B:2383:LYS:NZ	6:B:2604:DDS:O3A	2.54	0.40
1:C:1994:TRP:NE1	1:C:1998:PRO:HA	2.36	0.40
1:C:2210:VAL:HG21	1:C:2253:PRO:HG3	2.04	0.40
1:B:1855:ALA:HB1	1:B:2045:ARG:NH2	2.37	0.40
1:C:2256:PHE:CZ	1:C:2312:ILE:HD11	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2058:ASN:ND2	3:K:18:DG:O3'[2_555]	2.16	0.04

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	613/799 (77%)	541 (88%)	66 (11%)	6 (1%)	15	52
1	B	613/799 (77%)	541 (88%)	67 (11%)	5 (1%)	19	57
1	C	613/799 (77%)	541 (88%)	67 (11%)	5 (1%)	19	57
1	D	613/799 (77%)	545 (89%)	63 (10%)	5 (1%)	19	57
All	All	2452/3196 (77%)	2168 (88%)	263 (11%)	21 (1%)	17	54

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2124	SER

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Mol	Chain	Res	Type
1	B	2124	SER
1	D	1957	ASP
1	A	1954	LYS
1	A	1957	ASP
1	A	2135	GLU
1	B	1954	LYS
1	B	1957	ASP
1	B	2144	PRO
1	C	1957	ASP
1	D	1954	LYS
1	D	2135	GLU
1	A	2144	PRO
1	B	1859	ILE
1	C	1954	LYS
1	C	2144	PRO
1	A	1859	ILE
1	C	1859	ILE
1	D	1859	ILE
1	D	2144	PRO
1	A	2246	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/699 (79%)	537 (98%)	14 (2%)	47	69
1	B	551/699 (79%)	537 (98%)	14 (2%)	47	69
1	C	551/699 (79%)	538 (98%)	13 (2%)	49	69
1	D	551/699 (79%)	535 (97%)	16 (3%)	42	65
All	All	2204/2796 (79%)	2147 (97%)	57 (3%)	46	68

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1826	SER

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Mol	Chain	Res	Type
1	A	1854	LEU
1	A	1857	GLU
1	A	1858	LYS
1	A	1977	SER
1	A	2177	PHE
1	A	2182	ASP
1	A	2236	HIS
1	A	2245	THR
1	A	2424	ASN
1	A	2470	ASN
1	A	2537	GLN
1	A	2566	VAL
1	A	2582	TRP
1	B	1826	SER
1	B	1854	LEU
1	B	1857	GLU
1	B	1858	LYS
1	B	1977	SER
1	B	2141	LEU
1	B	2177	PHE
1	B	2245	THR
1	B	2416	PHE
1	B	2424	ASN
1	B	2470	ASN
1	B	2537	GLN
1	B	2566	VAL
1	B	2582	TRP
1	C	1826	SER
1	C	1854	LEU
1	C	1857	GLU
1	C	1858	LYS
1	C	1943	ASP
1	C	1977	SER
1	C	2177	PHE
1	C	2182	ASP
1	C	2245	THR
1	C	2424	ASN
1	C	2470	ASN
1	C	2566	VAL
1	C	2582	TRP
1	D	1826	SER
1	D	1854	LEU

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Mol	Chain	Res	Type
1	D	1858	LYS
1	D	1943	ASP
1	D	1977	SER
1	D	2061	ASN
1	D	2141	LEU
1	D	2177	PHE
1	D	2182	ASP
1	D	2236	HIS
1	D	2245	THR
1	D	2424	ASN
1	D	2470	ASN
1	D	2537	GLN
1	D	2566	VAL
1	D	2582	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1984	GLN
1	A	2027	GLN
1	A	2205	ASN
1	B	1984	GLN
1	B	2380	GLN
1	C	1984	GLN
1	C	2380	GLN
1	D	1969	GLN
1	D	1984	GLN
1	D	2061	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	DDS	A	2604	5	25,31,31	0.95	1 (4%)	26,48,48	1.48	4 (15%)
4	GOL	D	2601	-	5,5,5	0.36	0	5,5,5	0.38	0
6	DDS	C	2604	5	25,31,31	0.95	1 (4%)	26,48,48	1.64	6 (23%)
4	GOL	B	2601	-	5,5,5	0.33	0	5,5,5	0.58	0
4	GOL	D	2602	-	5,5,5	0.37	0	5,5,5	0.32	0
6	DDS	B	2604	5	25,31,31	0.87	1 (4%)	26,48,48	1.40	3 (11%)
4	GOL	B	2602	-	5,5,5	0.39	0	5,5,5	0.31	0
6	DDS	D	2604	5	25,31,31	0.90	1 (4%)	26,48,48	1.59	4 (15%)
4	GOL	C	2602	-	5,5,5	0.39	0	5,5,5	0.28	0
4	GOL	A	2602	-	5,5,5	0.38	0	5,5,5	0.46	0
4	GOL	A	2601	-	5,5,5	0.35	0	5,5,5	0.39	0
4	GOL	C	2601	-	5,5,5	0.33	0	5,5,5	0.43	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
6	DDS	A	2604	5	-	5/18/31/31	0/3/3/3
4	GOL	D	2601	-	-	2/4/4/4	-
6	DDS	C	2604	5	-	4/18/31/31	0/3/3/3
4	GOL	B	2601	-	-	2/4/4/4	-
4	GOL	D	2602	-	-	2/4/4/4	-
6	DDS	B	2604	5	-	5/18/31/31	0/3/3/3
4	GOL	B	2602	-	-	2/4/4/4	-
6	DDS	D	2604	5	-	3/18/31/31	0/3/3/3
4	GOL	C	2602	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	2602	-	-	2/4/4/4	-
4	GOL	A	2601	-	-	2/4/4/4	-
4	GOL	C	2601	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2604	DDS	C2-N3	2.78	1.36	1.32
6	A	2604	DDS	C2-N3	2.38	1.35	1.32
6	B	2604	DDS	C2-N3	2.29	1.35	1.32
6	C	2604	DDS	C5-N7	-2.17	1.31	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	2604	DDS	PB-O3A-PA	-4.27	118.17	132.83
6	C	2604	DDS	PB-O3A-PA	-4.26	118.21	132.83
6	D	2604	DDS	PB-O3B-PG	-4.00	119.09	132.83
6	A	2604	DDS	PB-O3A-PA	-3.96	119.25	132.83
6	A	2604	DDS	PB-O3B-PG	-3.85	119.60	132.83
6	B	2604	DDS	PB-O3A-PA	-3.66	120.26	132.83
6	B	2604	DDS	PB-O3B-PG	-3.32	121.43	132.83
6	C	2604	DDS	C4'-O4'-C1'	2.92	112.57	109.81
6	C	2604	DDS	PB-O3B-PG	-2.90	122.86	132.83
6	C	2604	DDS	C3'-C2'-C1'	2.60	105.78	102.78
6	A	2604	DDS	C5-C6-N6	2.46	124.09	120.35
6	B	2604	DDS	C5-C6-N6	2.41	124.02	120.35
6	D	2604	DDS	C5-C6-N6	2.33	123.89	120.35
6	C	2604	DDS	C5-C6-N6	2.32	123.88	120.35
6	C	2604	DDS	C4-C5-N7	2.09	111.58	109.40
6	A	2604	DDS	C4-C5-N7	2.05	111.54	109.40
6	D	2604	DDS	C4'-O4'-C1'	2.02	111.72	109.81

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2604	DDS	PB-O3A-PA-O5'
6	A	2604	DDS	C5'-O5'-PA-O2A
6	A	2604	DDS	C5'-O5'-PA-O3A

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Mol	Chain	Res	Type	Atoms
4	D	2601	GOL	O1-C1-C2-C3
6	C	2604	DDS	C5'-O5'-PA-O1A
6	C	2604	DDS	C5'-O5'-PA-O2A
4	D	2602	GOL	O1-C1-C2-C3
6	B	2604	DDS	C5'-O5'-PA-O2A
6	B	2604	DDS	C5'-O5'-PA-O3A
6	B	2604	DDS	O4'-C4'-C5'-O5'
4	B	2602	GOL	O1-C1-C2-C3
6	D	2604	DDS	C5'-O5'-PA-O1A
6	D	2604	DDS	C5'-O5'-PA-O2A
4	C	2602	GOL	O1-C1-C2-C3
4	A	2602	GOL	O1-C1-C2-C3
4	A	2601	GOL	O1-C1-C2-C3
4	C	2601	GOL	O1-C1-C2-C3
6	A	2604	DDS	O4'-C4'-C5'-O5'
4	B	2601	GOL	O1-C1-C2-C3
4	D	2601	GOL	O1-C1-C2-O2
4	C	2602	GOL	O1-C1-C2-O2
4	A	2601	GOL	O1-C1-C2-O2
4	B	2601	GOL	O1-C1-C2-O2
4	D	2602	GOL	O1-C1-C2-O2
4	C	2601	GOL	O1-C1-C2-O2
4	B	2602	GOL	O1-C1-C2-O2
4	A	2602	GOL	O1-C1-C2-O2
6	A	2604	DDS	C3'-C4'-C5'-O5'
6	B	2604	DDS	C3'-C4'-C5'-O5'
6	C	2604	DDS	PA-O3A-PB-O1B
6	C	2604	DDS	C5'-O5'-PA-O3A
6	D	2604	DDS	C5'-O5'-PA-O3A
6	B	2604	DDS	PA-O3A-PB-O1B

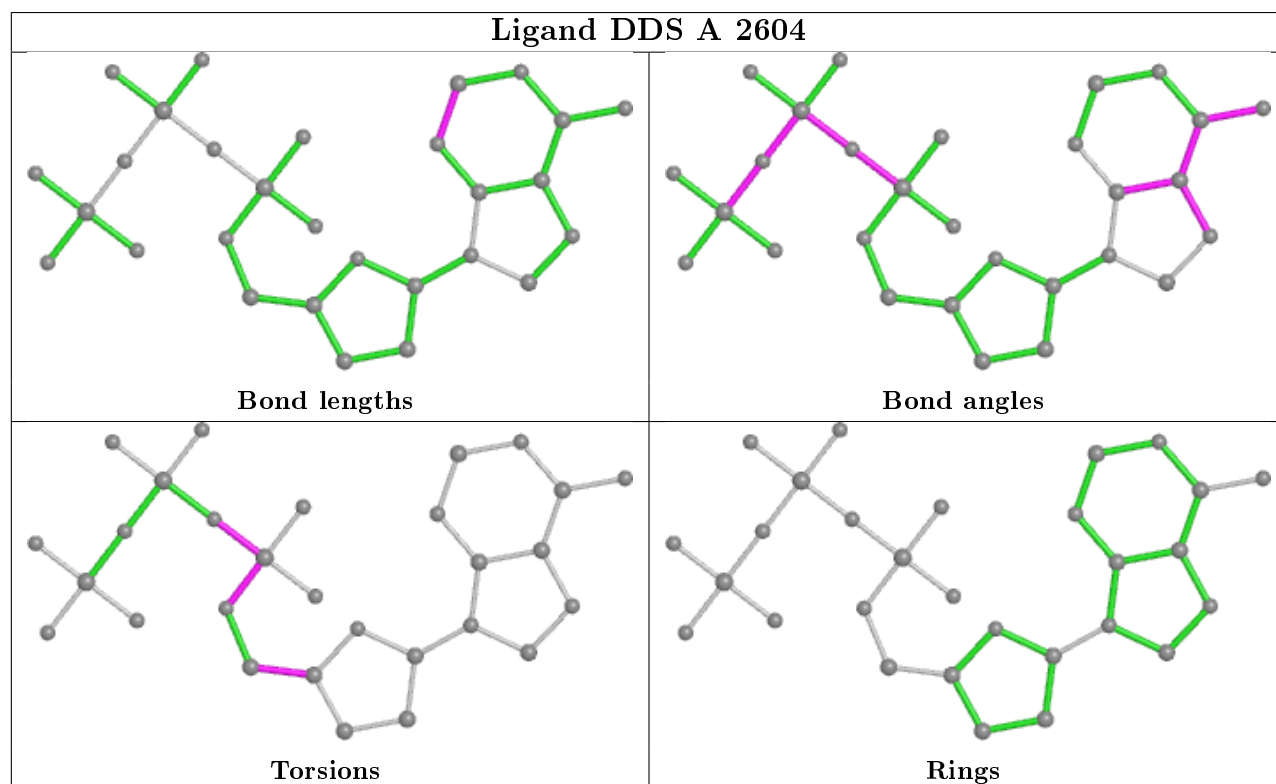
There are no ring outliers.

5 monomers are involved in 24 short contacts:

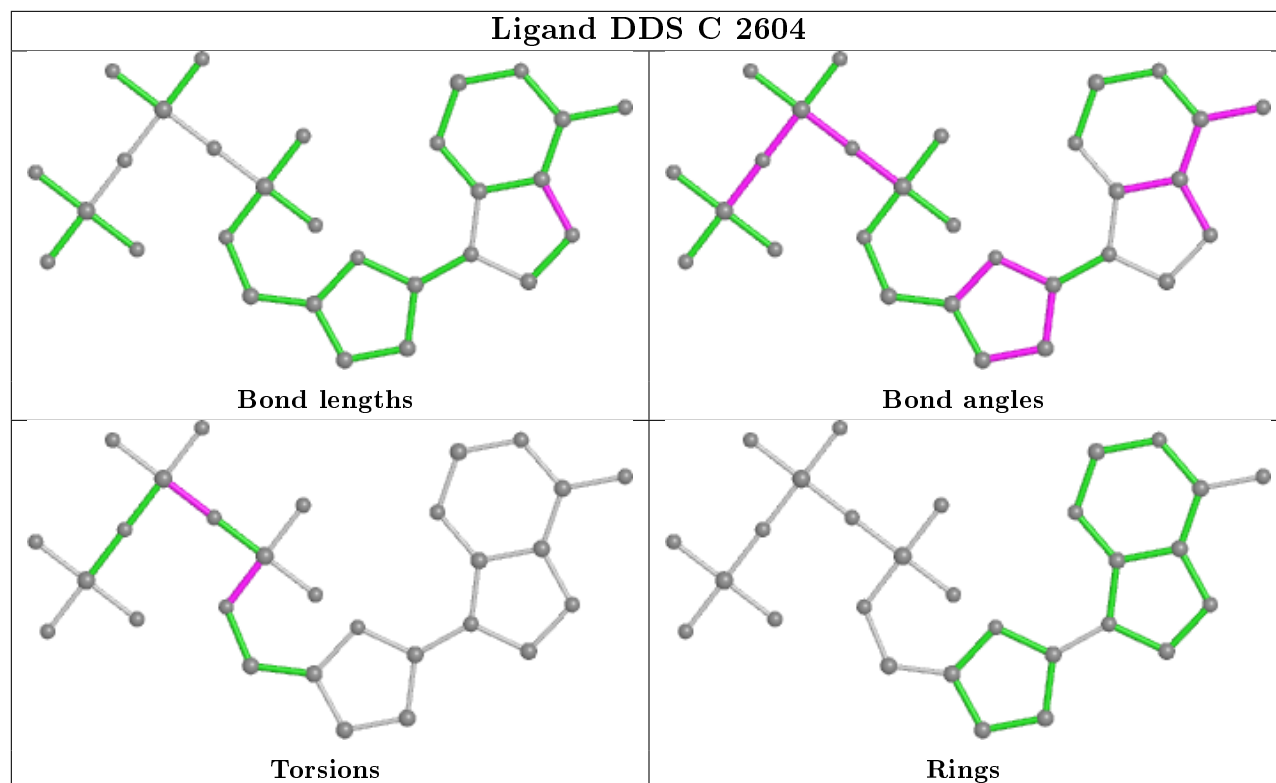
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	2604	DDS	4	0
6	C	2604	DDS	4	0
6	B	2604	DDS	9	0
4	B	2602	GOL	1	0
6	D	2604	DDS	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

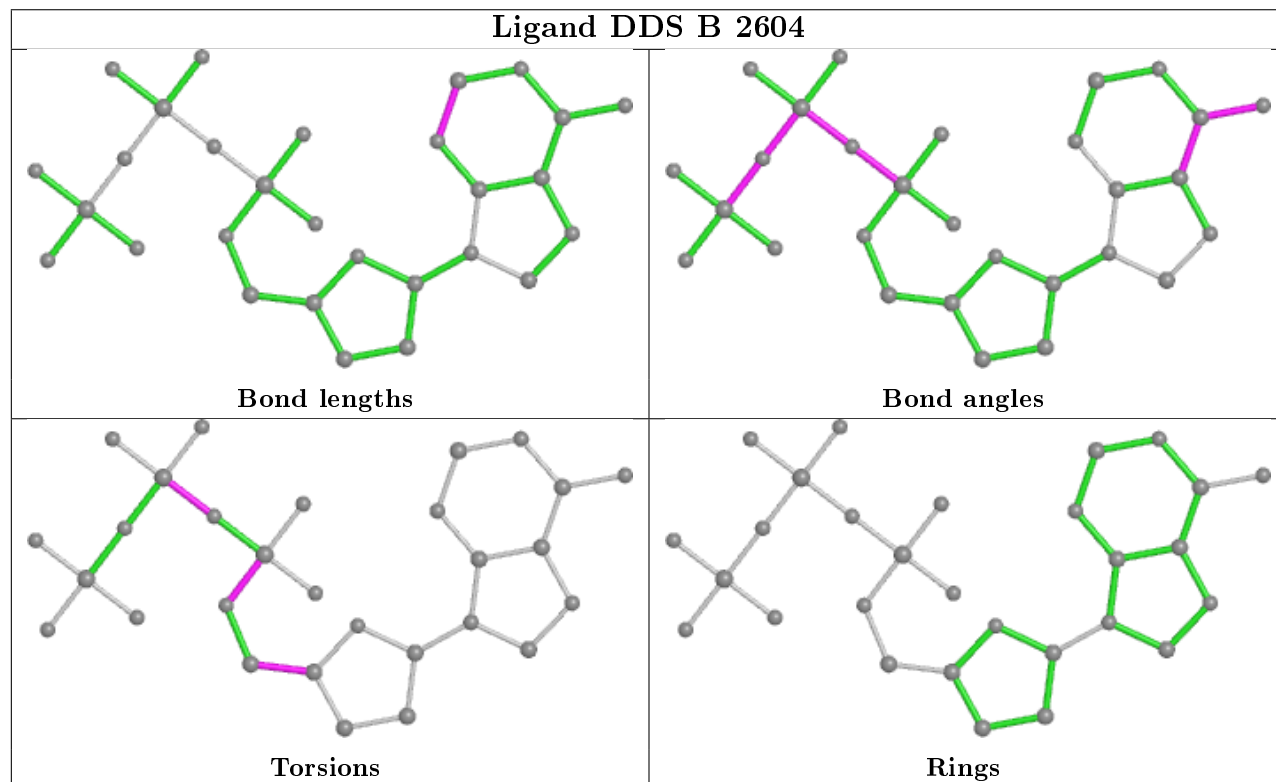
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

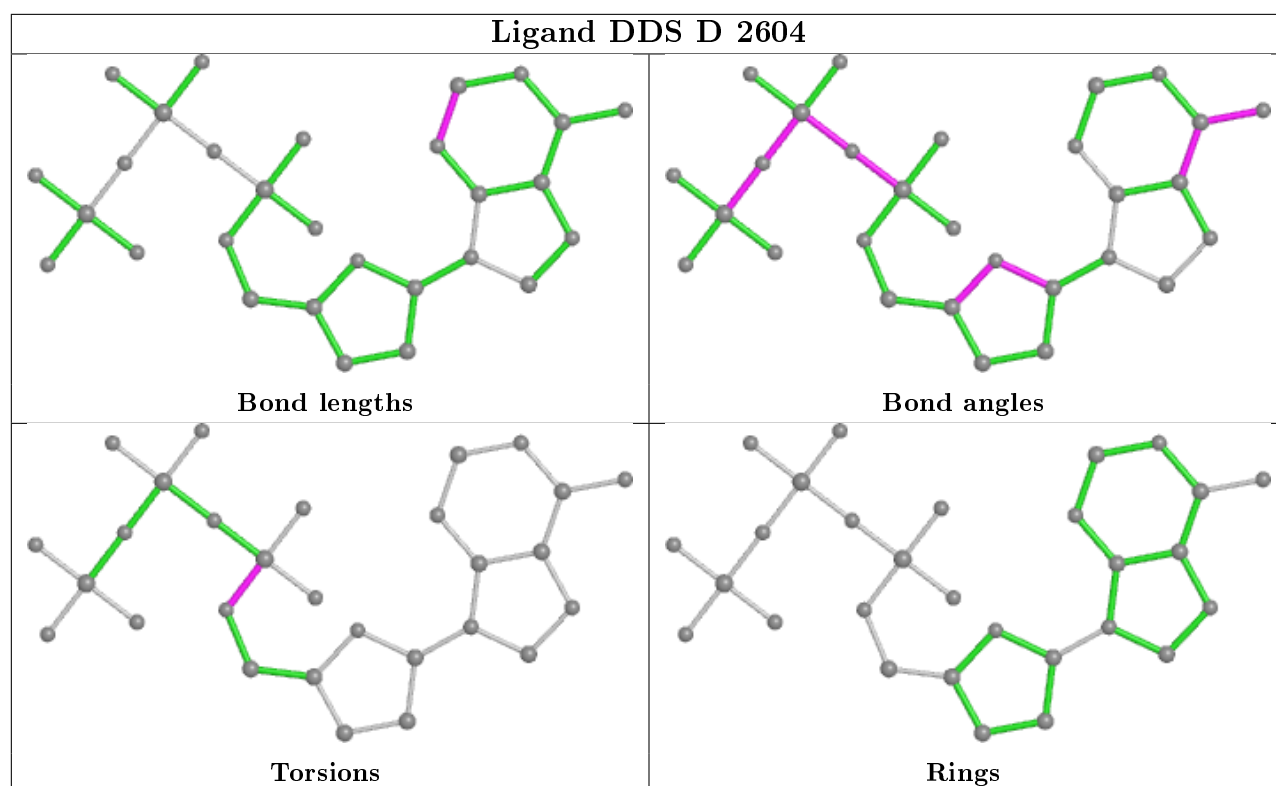


Ligand DDS C 2604



Ligand DDS B 2604





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, 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	625/799 (78%)	0.10	24 (3%)	40	32	86, 160, 254, 348	0
1	B	625/799 (78%)	0.20	30 (4%)	30	26	85, 173, 289, 424	0
1	C	625/799 (78%)	0.41	48 (7%)	13	11	106, 197, 293, 360	0
1	D	625/799 (78%)	0.36	48 (7%)	13	11	113, 209, 303, 364	0
2	F	12/13 (92%)	-0.49	0	100	100	148, 188, 247, 277	0
2	H	13/13 (100%)	-0.08	0	100	100	169, 237, 333, 351	0
2	J	12/13 (92%)	-0.20	0	100	100	146, 209, 272, 279	0
2	L	13/13 (100%)	-0.22	0	100	100	170, 206, 272, 322	0
3	E	18/18 (100%)	0.63	2 (11%)	5	5	140, 182, 297, 302	0
3	G	18/18 (100%)	0.40	0	100	100	145, 229, 363, 369	0
3	I	18/18 (100%)	0.34	0	100	100	131, 213, 284, 298	0
3	K	18/18 (100%)	-0.14	0	100	100	156, 203, 258, 269	0
All	All	2622/3320 (78%)	0.26	152 (5%)	23	19	85, 188, 289, 424	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2590	VAL	7.6
1	B	2589	ASP	6.7
1	C	2590	VAL	6.6
1	B	2036	ALA	5.7
1	C	2120	LEU	5.6
1	C	2196	LEU	5.6
1	D	2193	LEU	5.5
1	B	2307	GLY	5.5
1	D	2120	LEU	5.5
1	B	2176	GLN	5.3
1	C	2307	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	C	1830	VAL	4.9
3	E	18	DG	4.7
1	A	2309	PRO	4.6
1	D	2189	ALA	4.4
1	C	2125	PHE	4.4
1	D	2532	GLY	4.3
1	D	2023	MET	4.3
1	C	2039	GLU	4.2
1	C	2043	ARG	4.2
1	B	2325	SER	4.2
1	C	1856	CYS	4.2
1	C	2531	GLY	4.1
1	C	2044	TYR	4.0
1	C	2127	PHE	4.0
1	D	2192	PRO	4.0
1	B	2512	ASP	4.0
1	D	2510	GLN	3.9
1	D	2307	GLY	3.8
1	C	2126	SER	3.8
1	C	2512	ASP	3.8
1	D	2218	LYS	3.8
1	D	2531	GLY	3.8
1	D	2119	GLN	3.8
1	C	2199	GLU	3.7
1	A	2142	LYS	3.7
1	C	2023	MET	3.6
1	A	2310	PHE	3.6
1	D	2512	ASP	3.6
1	C	2308	MET	3.5
1	C	1913	TYR	3.5
1	B	2178	SER	3.4
1	D	2116	GLN	3.4
1	D	2402	MET	3.3
1	D	2145	PRO	3.3
1	B	2590	VAL	3.3
1	C	2453	ILE	3.2
1	D	2025	THR	3.2
1	D	2215	GLN	3.2
1	D	2188	LYS	3.2
1	D	2194	PRO	3.1
1	A	2260	MET	3.1
1	A	2176	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	2140	GLU	3.0
1	D	2393	MET	3.0
1	B	2106	MET	3.0
1	C	1903	LEU	3.0
1	D	2187	LEU	3.0
1	A	2311	SER	2.9
1	B	2138	PHE	2.9
1	D	2511	SER	2.9
1	C	2182	ASP	2.9
1	D	2182	ASP	2.8
1	C	1916	SER	2.8
1	B	2136	VAL	2.8
1	A	2143	LEU	2.8
1	C	2208	THR	2.8
1	C	2038	SER	2.8
1	C	2314	MET	2.8
1	C	1834	GLN	2.8
1	A	2452	GLY	2.8
1	D	1834	GLN	2.7
1	D	1912	ALA	2.7
1	C	1831	ALA	2.7
1	D	2141	LEU	2.7
1	C	2310	PHE	2.7
1	D	2020	LEU	2.7
1	B	1935	LEU	2.7
1	C	2193	LEU	2.6
1	B	2218	LYS	2.6
1	D	2127	PHE	2.6
1	C	2134	ALA	2.6
1	B	2139	LEU	2.6
1	B	2145	PRO	2.6
1	D	2589	ASP	2.6
1	B	2120	LEU	2.5
1	D	2453	ILE	2.5
1	A	2145	PRO	2.5
1	C	1829	ASP	2.5
1	A	1827	ILE	2.5
1	C	2040	HIS	2.5
1	C	2197	ILE	2.5
1	C	1915	PHE	2.5
1	A	2512	ASP	2.5
1	B	2314	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	2106	MET	2.4
1	D	2327	LEU	2.4
1	C	2001	GLN	2.4
1	D	2329	ALA	2.4
1	D	1825	LEU	2.4
1	C	2200	TRP	2.4
1	D	2455	ASP	2.4
1	D	2325	SER	2.4
1	C	1902	GLY	2.3
1	C	2124	SER	2.3
1	A	2138	PHE	2.3
1	D	2580	ALA	2.3
1	A	2140	GLU	2.3
1	B	2035	ASN	2.3
1	C	2002	GLU	2.3
1	A	2308	MET	2.2
1	D	2006	HIS	2.2
1	B	2424	ASN	2.2
1	D	1913	TYR	2.2
1	B	2025	THR	2.2
1	B	2033	GLY	2.2
1	B	2125	PHE	2.2
1	C	1914	TYR	2.2
1	C	2106	MET	2.2
1	C	2013	LEU	2.2
1	C	2144	PRO	2.2
1	B	2368	MET	2.2
1	B	2109	LYS	2.2
1	A	2258	ILE	2.1
1	A	2259	LYS	2.1
1	C	2218	LYS	2.1
1	B	2128	THR	2.1
1	A	2194	PRO	2.1
3	E	17	DC	2.1
1	D	1965	TYR	2.1
1	D	2036	ALA	2.1
1	A	1901	VAL	2.1
1	C	2178	SER	2.1
1	B	2387	TYR	2.1
1	A	2257	GLU	2.1
1	D	2196	LEU	2.1
1	C	1838	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	2326	ILE	2.1
1	D	2309	PRO	2.1
1	A	2314	MET	2.1
1	B	1824	SER	2.1
1	D	2452	GLY	2.1
1	D	2559	LYS	2.0
1	D	1827	ILE	2.0
1	A	2117	ALA	2.0
1	D	2111	ASP	2.0
1	C	2258	ILE	2.0
1	A	2141	LEU	2.0
1	A	2036	ALA	2.0
1	B	1965	TYR	2.0
1	A	2023	MET	2.0
1	B	2407	ASN	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 carbohydrates 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.

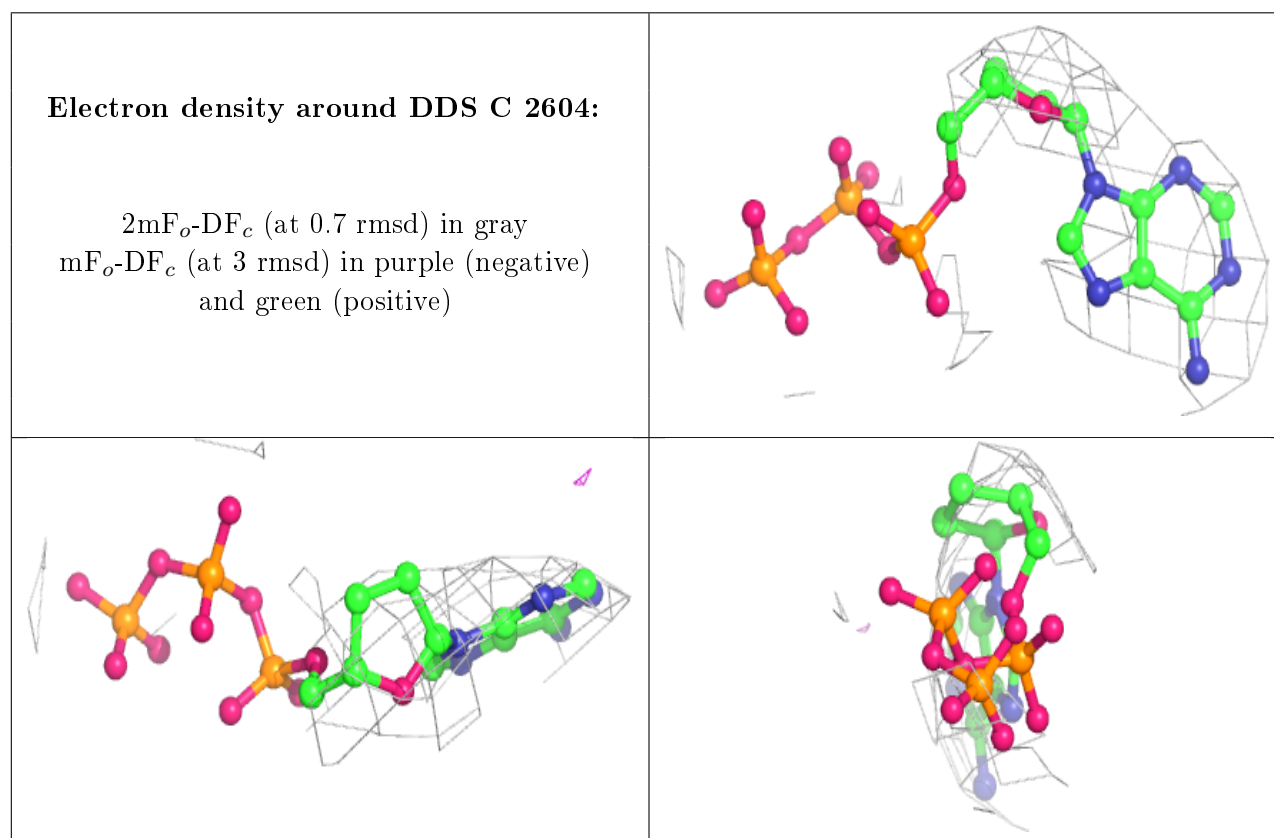
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	B	2601	6/6	0.19	0.55	191,207,209,214	0
4	GOL	D	2601	6/6	0.41	0.51	126,149,162,182	0
4	GOL	A	2601	6/6	0.50	0.62	123,156,159,172	0
4	GOL	C	2601	6/6	0.58	0.49	143,164,171,173	0
4	GOL	A	2602	6/6	0.75	0.76	110,124,138,146	0
4	GOL	C	2602	6/6	0.82	0.46	102,104,115,116	0
5	CA	D	2603	1/1	0.83	0.29	226,226,226,226	0
4	GOL	B	2602	6/6	0.89	0.38	98,111,113,119	0

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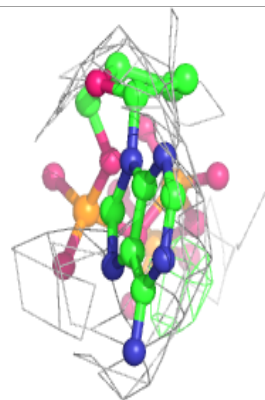
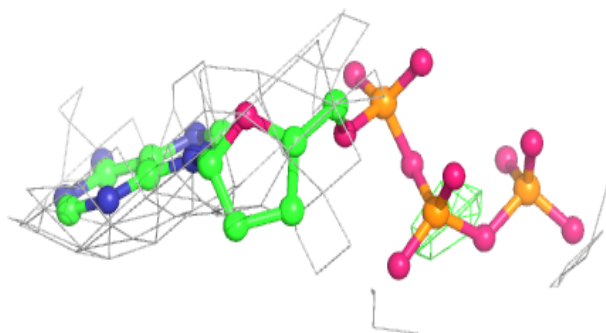
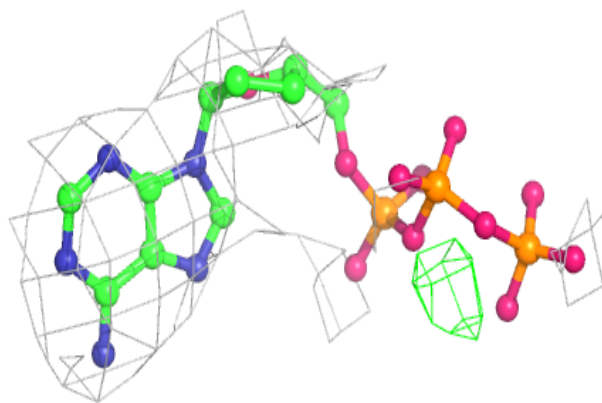
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	D	2602	6/6	0.91	0.50	112,118,123,124	0
6	DDS	C	2604	29/29	0.92	0.28	157,166,243,249	0
6	DDS	A	2604	29/29	0.94	0.27	168,190,205,209	0
6	DDS	D	2604	29/29	0.94	0.28	201,209,239,250	0
6	DDS	B	2604	29/29	0.94	0.33	217,221,257,278	0
5	CA	A	2603	1/1	0.95	0.20	187,187,187,187	0
5	CA	B	2603	1/1	0.96	0.30	223,223,223,223	0
5	CA	C	2603	1/1	0.97	0.23	289,289,289,289	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.

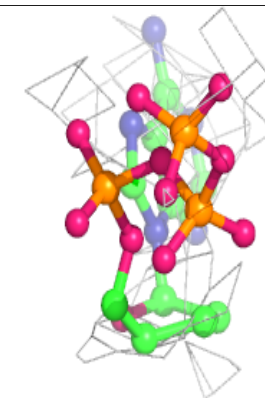
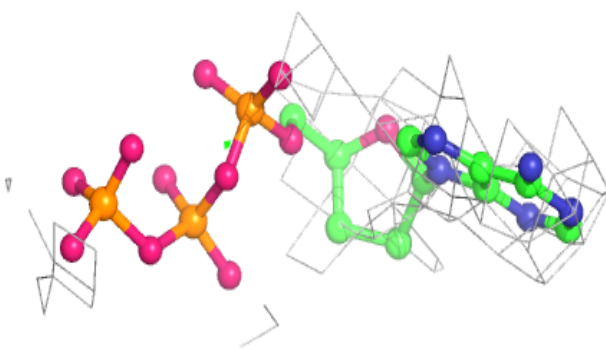
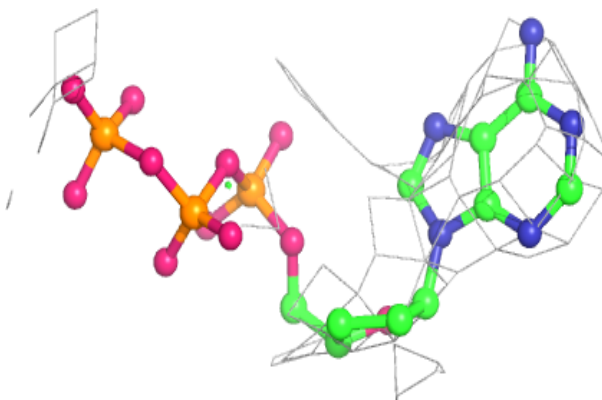


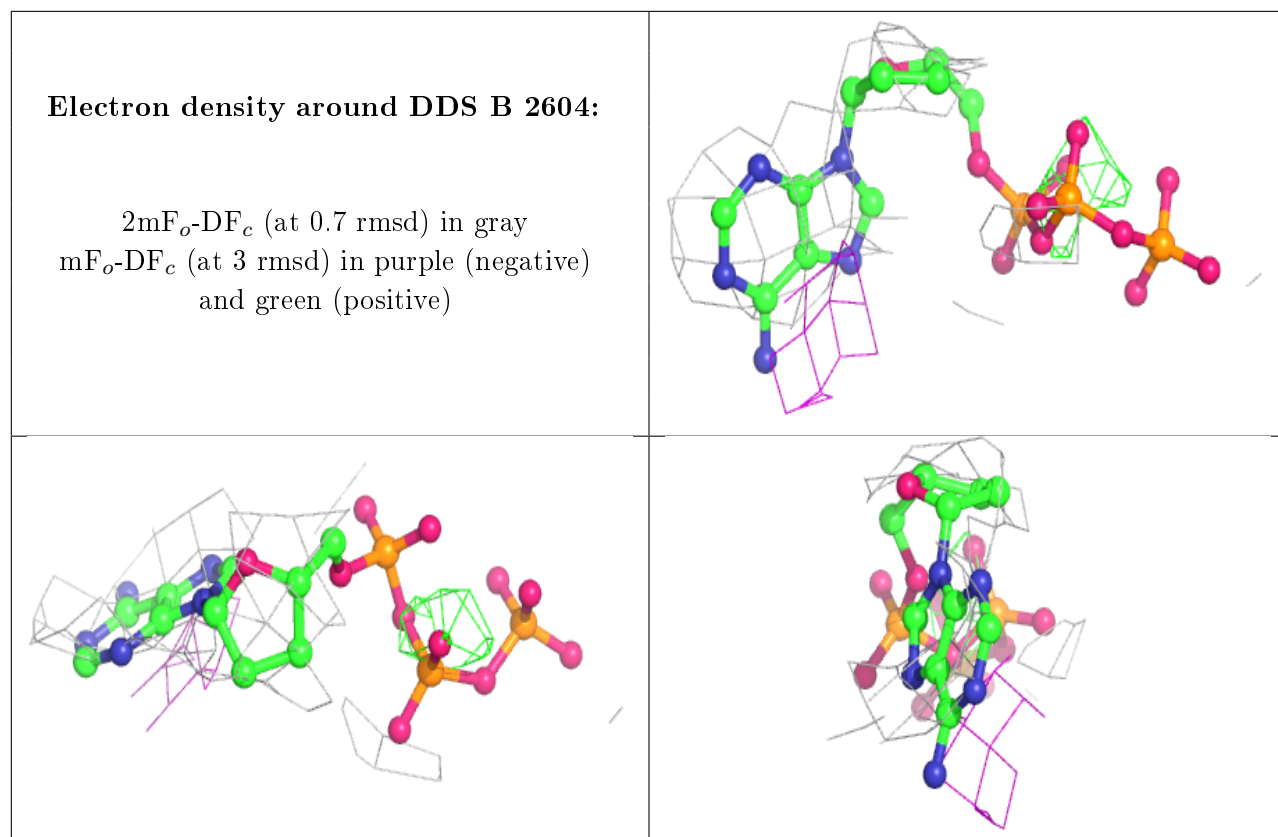
Electron density around DDS A 2604:

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

**Electron density around DDS D 2604:**

$2mF_o-DF_c$ (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.