



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2018 – 04:39 am GMT

PDB ID : 4X0Q
Title : Ternary complex of human DNA polymerase theta C-terminal domain binding ddGTP opposite dCMP
Authors : Zahn, K.E.; Doubie, S.
Deposited on : 2014-11-22
Resolution : 3.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk31020
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk31020

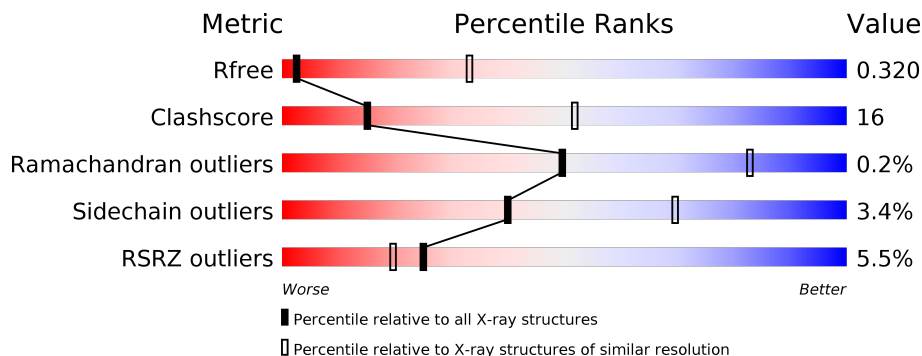
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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}	111664	1145 (4.20-3.60)
Clashscore	122126	1225 (4.20-3.60)
Ramachandran outliers	120053	1184 (4.20-3.60)
Sidechain outliers	120020	1175 (4.20-3.60)
RSRZ outliers	108989	1046 (4.20-3.60)

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. 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	772	<div> <div>4%</div> <div> <div>51%</div> <div>29%</div> <div>•</div> <div>19%</div> </div> </div>
1	B	772	<div> <div>5%</div> <div> <div>53%</div> <div>27%</div> <div>•</div> <div>19%</div> </div> </div>
2	E	17	<div> <div>6%</div> <div> <div>24%</div> <div>53%</div> <div>24%</div> </div> </div>
2	G	17	<div> <div>6%</div> <div> <div>6%</div> <div>65%</div> <div>6%</div> <div>24%</div> </div> </div>
3	F	13	<div> <div>31%</div> <div>38%</div> <div>31%</div> </div>
3	H	13	<div> <div>8%</div> <div> <div>31%</div> <div>38%</div> <div>31%</div> </div> </div>

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	B	2601	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10902 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			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	13	Total	C	N	O	P	0	0	0
			263	126	51	74	12			
2	G	13	Total	C	N	O	P	0	0	0
			263	126	51	74	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	9	Total	C	N	O	P	0	0	0
			182	88	29	56	9			
3	H	9	Total	C	N	O	P	0	0	0
			182	88	29	56	9			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

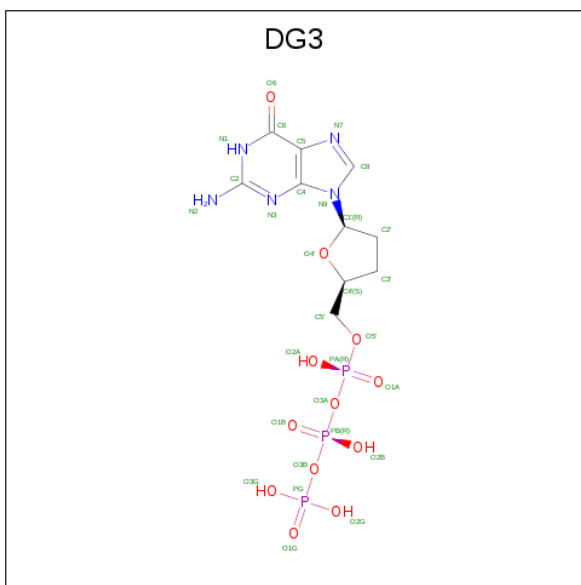


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 6 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (three-letter code: DG3) (formula: C₁₀H₁₆N₅O₁₂P₃).



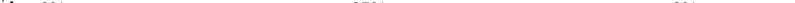
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
6	B	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Chain B:

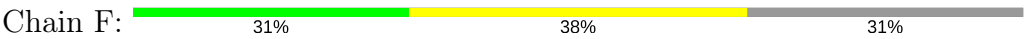
5% 53% 27% 19%

LYS	M2402	ASW	V2232	SER	V2072	GLY	SER	S1824
LEU	F2416	PRO	G2233	THR	Q2081	PHE	THR	L1825
GLN	N2424	ARG	G2234	ARG	L2084	SER	ARG	S1826
PHE	M2427	GLN	H2236	GLY	Q2077	ILE	GLY	I1827
G2527	G2531	GLN	T2237	ASP	L1975	GLY	CYS	D1833
G2532	T2430	MET	A2238	ASN	L1976	GLY	THR	I1834
F2533	Q2441	GLU	T2239	GLY	S1977	GLY	THR	N1835
F2534	Q2442	ARG	G2240	LYS	L2087	GLY	THR	I1836
I2535	T2443	ALA	T2241	LEU	E2088	GLY	THR	F1837
L2536	L2444	ALA	T2242	LEU	L2089	GLY	THR	F1840
Q2537	L2445	ASP	T2243	ARG	N2090	GLY	THR	I1844
L2538	G2445	ASP	T2244	LEU	G2091	GLY	THR	K1848
M2539	Q2448	G2307	E2245	ARG	I2092	GLY	THR	R1849
D2540	P2448	P2247	P2247	Q2176	G2093	GLY	THR	I1852
E2541	F2309	N2248	N2248	F2177	L2096	GLN	THR	S1853
L2542	F2310	I2249	I2249	S2178	T2096	LYS	THR	L1854
L2543	S2311	Q2250	Q2250	S2179	Q2102	GLY	THR	A1855
L2544	S2312	N2251	N2251	S2180	I2105	GLN	THR	C1856
L2545	Q2313	V2252	V2252	V2183	I2106	LYS	THR	E1857
E2546	M2314	D2255	D2255	L2184	K2109	HIS	THR	K1858
A2547	H2463	F2256	F2256	N2185	K2109	SER	THR	I1859
Q2553	Q2467	E2257	E2257	K2186	I2113	SER	THR	R1860
V2556	P2468	G2258	G2258	L2187	I2113	GLY	THR	SER
K2557	I2469	K2259	K2259	K2188	A2117	ILE	THR	LYS
L2566	N2470	M2260	M2260	A2189	L2120	ALA	THR	ALA
S2569	V2473	PRO	PRO	L2190	H2191	SER	THR	VAL
V2570	S2476	THR	THR	H2192	L2192	LEU	THR	PRO
K2575	V2481	GLY	GLY	L2193	F2125	PRO	THR	LEU
K2577	K2482	SER	SER	G2195	I2133	SER	THR	THR
S2581	I2483	PRO	PRO	L2196	E2134	SER	THR	SER
G2582	A2484	GLN	GLN	L2197	E2135	LYS	THR	LYS
G2583	T2485	SER	SER	L2198	V2136	THR	THR	ALA
E2584	I2488	ALA	ALA	T2203	L2137	THR	THR	ALA
L2585	F2499	I2349	I2349	T2204	F2138	THR	THR	ILE
K2586	K2500	GLY	GLY	L2205	E2140	GLY	THR	GLY
D2587	H2504	LEU	LEU	F2212	L2141	ARG	THR	ARG
F2588	E2505	LEU	LEU	P2213	P2144	ASN	THR	LYS
D2589	M2508	PRO	PRO	P2213	ASN	ARG	THR	LYS
V2590	D2512	MET	MET	R2216	GLY	ARG	THR	GLN
	THR	ARG	ARG	E2217	GLY	GLY	THR	ALA
	GLY	LYS	LYS	K2218	MET	LYS	THR	ALA
	LEU	GLY	GLY	C2219	ASN	GLN	THR	SER
	SER	LYS	LYS	L2220	ASN	GLY	THR	SER
	ARG	THR	THR	N2221	GLY	GLY	THR	PRO
	LYS	LYS	LYS	P2222	SER	LYS	THR	GLY
	LYS	PHE	PHE	L2224	THR	THR	THR	ILE
	ARG	VAL	VAL	E2227	LEU	LEU	THR	ARG
	ARG	VAL	VAL	P2228	GLY	GLY	THR	ASP

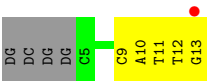
- Chain E:  6% 24% 53% 17%

- Chain G: 

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	99.70Å 135.39Å 159.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.93 – 3.90 39.82 – 3.85	Depositor EDS
% Data completeness (in resolution range)	82.5 (29.93-3.90) 82.6 (39.82-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.87Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.258 , 0.316 0.262 , 0.320	Depositor DCC
R_{free} test set	877 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	102.3	Xtriage
Anisotropy	0.997	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	10902	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 42.70 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.9642e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, MG, DG3

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	0.31	0/5056	0.57	0/6818
1	B	0.30	0/5056	0.57	0/6818
2	E	0.57	0/295	0.87	0/453
2	G	0.57	0/295	0.88	1/453 (0.2%)
3	F	0.60	0/202	1.07	0/309
3	H	0.63	0/202	1.04	0/309
All	All	0.34	0/11106	0.62	1/15160 (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
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	5	DC	O4'-C1'-N1	5.12	111.58	108.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1953	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	2245	THR	Peptide
1	A	2583	GLY	Peptide
1	B	1953	ARG	Peptide
1	B	2245	THR	Peptide
1	B	2246	GLU	Peptide
1	B	2583	GLY	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	4963	0	4980	156	0
1	B	4963	0	4980	157	0
2	E	263	0	147	12	0
2	G	263	0	147	14	0
3	F	182	0	102	9	0
3	H	182	0	102	6	0
4	A	12	0	16	3	0
4	B	12	0	16	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	30	0	12	4	0
6	B	30	0	12	4	0
All	All	10902	0	10514	345	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 16.

All (345) 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:2030:GLN:HB3	1:A:2045:ARG:HB3	1.53	0.91
1:A:1857:GLU:HB3	1:A:1858:LYS:HD3	1.55	0.88
1:B:2030:GLN:HB3	1:B:2045:ARG:HB3	1.56	0.87
1:A:1968:ILE:HD13	1:A:2233:SER:HB3	1.57	0.86
1:B:1968:ILE:HD13	1:B:2233:SER:HB3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2004:THR:HB	1:B:2026:SER:HB3	1.60	0.83
1:A:2243:THR:HG21	2:E:7:DA:H2''	1.64	0.80
6:A:2604:DG3:O1B	6:A:2604:DG3:O1A	1.96	0.79
6:B:2604:DG3:O1B	6:B:2604:DG3:O1A	1.98	0.79
2:E:10:DA:H2''	2:E:11:DC:H5''	1.64	0.79
1:B:2581:SER:OG	1:B:2582:TRP:N	2.17	0.78
1:B:2248:ASN:HD22	2:G:8:DT:H4'	1.47	0.78
2:E:11:DC:H2''	2:E:12:DA:H5''	1.70	0.73
2:G:11:DC:H2''	2:G:12:DA:H5''	1.70	0.73
1:A:2315:ARG:HB2	1:A:2582:TRP:CD1	2.24	0.73
6:A:2604:DG3:O1B	6:A:2604:DG3:O1G	2.06	0.72
1:A:2022:GLY:O	1:A:2040:HIS:NE2	2.22	0.72
1:B:1857:GLU:HB3	1:B:1858:LYS:HD3	1.72	0.72
2:G:9:DG:H2''	2:G:10:DA:C8	2.24	0.71
1:A:2004:THR:HB	1:A:2026:SER:HB3	1.71	0.71
1:A:2041:SER:HA	1:A:2045:ARG:HE	1.56	0.70
1:B:1965:TYR:HB3	1:B:2029:ILE:HG22	1.73	0.70
1:A:1948:LEU:HD22	1:A:1980:ILE:HD13	1.72	0.70
1:B:2041:SER:HA	1:B:2045:ARG:HE	1.57	0.70
2:E:9:DG:H2''	2:E:10:DA:C8	2.27	0.69
3:H:9:DC:H2'	3:H:10:DA:C8	2.27	0.69
1:B:2025:THR:HB	1:B:2036:ALA:HB3	1.76	0.68
1:B:2186:LYS:HE2	1:B:2194:PRO:HB3	1.76	0.68
1:B:1994:TRP:CD1	1:B:2236:HIS:HA	2.29	0.68
1:B:2193:LEU:HG	1:B:2196:LEU:HD13	1.74	0.68
1:A:2093:GLY:HA2	1:A:2228:ARG:HG2	1.75	0.67
1:B:1940:THR:O	1:B:1944:ARG:NH1	2.28	0.67
1:A:1963:VAL:HG11	1:A:2057:MET:HG2	1.77	0.66
2:G:10:DA:H2''	2:G:11:DC:H5''	1.77	0.66
1:A:2577:LYS:HG2	1:A:2586:LYS:HB2	1.78	0.65
3:F:9:DC:H2'	3:F:10:DA:C8	2.31	0.65
1:B:2187:LEU:HD11	1:B:2198:LEU:HD22	1.77	0.65
1:A:2470:ASN:HD21	2:E:6:DA:H5'	1.62	0.65
1:B:2535:ILE:HD11	1:B:2545:GLU:HB3	1.79	0.65
1:A:2535:ILE:HD11	1:A:2545:GLU:HB3	1.78	0.64
1:A:1965:TYR:HB3	1:A:2029:ILE:HG22	1.78	0.64
1:A:1994:TRP:CD1	1:A:2236:HIS:HA	2.33	0.63
6:B:2604:DG3:O1G	6:B:2604:DG3:O1B	2.16	0.63
1:A:2581:SER:OG	1:A:2582:TRP:N	2.22	0.62
1:B:2093:GLY:HA2	1:B:2228:ARG:HG2	1.82	0.62
1:A:1972:LYS:HG2	1:A:2089:LEU:HD21	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2604:DG3:O1A	6:A:2604:DG3:O1G	2.18	0.62
1:B:2243:THR:HG21	2:G:7:DA:H2"	1.81	0.61
1:A:1941:LEU:HD23	1:A:1944:ARG:HH12	1.65	0.61
1:B:1902:GLY:HA2	1:B:1917:LEU:HD13	1.81	0.61
1:A:2030:GLN:O	1:A:2045:ARG:NH1	2.34	0.60
1:B:1963:VAL:HG11	1:B:2057:MET:HG2	1.84	0.60
1:A:2568:LEU:HD12	1:A:2570:VAL:H	1.66	0.60
1:B:1963:VAL:HG12	1:B:1987:GLU:HB2	1.84	0.60
1:A:2208:THR:HA	1:A:2212:PHE:CD1	2.36	0.60
1:B:2109:LYS:HB2	1:B:2258:ILE:HD11	1.85	0.59
1:A:2102:GLN:NE2	1:A:2313:SER:O	2.33	0.59
2:G:12:DA:H2"	2:G:13:DG:H5"	1.85	0.58
1:A:2012:PHE:O	1:A:2014:PRO:HD3	2.03	0.58
1:A:2037:GLY:O	1:A:2041:SER:N	2.36	0.58
1:B:2102:GLN:NE2	1:B:2313:SER:O	2.33	0.58
1:A:2096:THR:OG1	1:A:2227:GLU:OE2	2.18	0.58
1:B:2538:LEU:HB2	1:B:2541:GLU:CB	2.34	0.58
1:A:2077:GLU:OE2	1:A:2482:LYS:NZ	2.36	0.58
1:B:1972:LYS:HG2	1:B:2089:LEU:HD21	1.85	0.57
1:A:2025:THR:HB	1:A:2036:ALA:HB3	1.85	0.57
1:A:1849:ARG:NH1	1:A:1987:GLU:OE1	2.37	0.57
1:B:1948:LEU:HD22	1:B:1980:ILE:HD13	1.86	0.57
1:A:2096:THR:OG1	1:A:2218:LYS:NZ	2.36	0.57
1:A:2243:THR:HA	1:A:2250:GLN:NE2	2.20	0.57
1:A:1848:LYS:O	1:A:1960:CYS:HB2	2.04	0.57
1:B:2084:LEU:HD11	1:B:2242:ILE:HD13	1.86	0.57
1:B:2077:GLU:OE2	1:B:2482:LYS:NZ	2.38	0.57
1:B:1834:GLN:HG2	1:B:1939:LEU:HD13	1.86	0.56
1:B:2022:GLY:O	1:B:2040:HIS:NE2	2.38	0.56
1:B:2241:ARG:HD3	1:B:2539:HIS:CE1	2.39	0.56
1:A:2474:GLN:NE2	2:E:5:DC:O2	2.38	0.56
1:B:1982:LEU:O	1:B:1986:TYR:OH	2.24	0.56
1:A:1940:THR:O	1:A:1944:ARG:NH1	2.39	0.56
1:B:1848:LYS:O	1:B:1960:CYS:HB2	2.06	0.55
1:B:2538:LEU:HB2	1:B:2541:GLU:HB2	1.88	0.55
1:A:1834:GLN:HG2	1:A:1939:LEU:HD13	1.87	0.55
1:A:2243:THR:HA	1:A:2250:GLN:HE22	1.70	0.55
1:B:2364:ALA:O	1:B:2369:ILE:HA	2.06	0.55
1:B:2568:LEU:HD12	1:B:2570:VAL:H	1.71	0.55
1:B:2213:PRO:O	1:B:2217:GLU:HG2	2.06	0.55
1:B:2087:LEU:HD12	1:B:2534:PHE:CE2	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2186:LYS:HE3	1:A:2190:LEU:HD23	1.89	0.55
1:B:2469:ILE:O	1:B:2473:VAL:HG12	2.07	0.55
1:A:2186:LYS:HE2	1:A:2194:PRO:HB3	1.90	0.54
1:A:2463:HIS:O	1:A:2467:GLN:HB2	2.07	0.54
1:B:2037:GLY:O	1:B:2041:SER:N	2.39	0.54
1:B:2444:LEU:HD21	1:B:2483:ILE:HD11	1.89	0.54
1:A:2248:ASN:HD22	2:E:8:DT:H4'	1.71	0.54
1:B:2012:PHE:O	1:B:2014:PRO:HD3	2.07	0.54
2:E:12:DA:H2''	2:E:13:DG:H5''	1.88	0.54
1:B:2216:ARG:NH2	1:B:2217:GLU:HB3	2.22	0.54
1:B:2251:ASN:HA	3:H:12:DT:H1'	1.90	0.54
1:A:2333:GLN:HB3	1:A:2336:LEU:HD12	1.89	0.54
1:B:1941:LEU:HD23	1:B:1944:ARG:HH12	1.73	0.54
1:B:1897:ASP:O	1:B:1977:SER:OG	2.26	0.54
1:A:2350:GLN:O	1:A:2354:THR:HG22	2.08	0.53
1:A:2338:ILE:HD11	1:A:2480:ILE:HD12	1.91	0.53
1:B:2245:THR:HA	1:B:2247:PRO:O	2.08	0.53
1:B:2577:LYS:HA	1:B:2586:LYS:HB2	1.90	0.53
1:A:1982:LEU:O	1:A:1986:TYR:OH	2.26	0.53
1:B:2047:SER:O	1:B:2051:ILE:HG22	2.09	0.53
1:A:2469:ILE:O	1:A:2473:VAL:HG12	2.09	0.53
1:A:2330:ASP:OD1	1:A:2331:TYR:O	2.26	0.53
1:B:1972:LYS:HD3	1:B:2088:GLU:OE1	2.09	0.53
1:B:2092:ILE:HB	1:B:2535:ILE:HG23	1.90	0.53
1:B:2481:VAL:HG21	1:B:2539:HIS:O	2.09	0.53
1:A:2141:LEU:HD22	1:A:2186:LYS:HZ2	1.74	0.53
1:A:1963:VAL:HG12	1:A:1987:GLU:HB2	1.91	0.52
1:B:2470:ASN:HD21	2:G:6:DA:H5'	1.75	0.52
1:B:2096:THR:OG1	1:B:2227:GLU:OE2	2.18	0.52
1:B:2243:THR:HA	1:B:2250:GLN:NE2	2.23	0.52
1:B:2087:LEU:HB2	1:B:2534:PHE:CD2	2.45	0.52
1:A:2208:THR:HA	1:A:2212:PHE:HD1	1.75	0.52
1:A:2321:PHE:HB2	1:A:2322:PRO:HD2	1.91	0.52
1:B:2232:VAL:O	1:B:2244:PHE:HA	2.09	0.52
1:B:2117:ALA:HA	1:B:2193:LEU:HD21	1.92	0.52
1:B:2220:LEU:HA	1:B:2227:GLU:HA	1.92	0.52
3:H:9:DC:H2'	3:H:10:DA:H8	1.73	0.52
1:A:2072:VAL:O	1:A:2076:VAL:HB	2.09	0.52
1:A:2364:ALA:O	1:A:2369:ILE:HA	2.09	0.52
1:A:2538:LEU:HB2	1:A:2541:GLU:CB	2.40	0.52
1:B:1965:TYR:HB2	1:B:2053:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2372:GLU:HG3	1:B:2373:SER:H	1.75	0.52
1:B:2096:THR:OG1	1:B:2218:LYS:NZ	2.40	0.51
1:B:2481:VAL:O	1:B:2485:THR:HG23	2.11	0.51
1:A:2538:LEU:HB2	1:A:2541:GLU:HB3	1.92	0.51
1:B:1983:GLU:O	1:B:1984:GLN:HG3	2.10	0.51
1:A:1901:VAL:HG23	1:A:1902:GLY:H	1.75	0.51
1:A:1852:ILE:HG12	1:A:1905:VAL:HG22	1.91	0.51
1:A:1943:ASP:N	1:A:1943:ASP:OD1	2.43	0.51
1:A:2245:THR:HA	1:A:2247:PRO:O	2.10	0.51
1:A:2087:LEU:HD12	1:A:2534:PHE:CE2	2.45	0.51
1:A:2184:LEU:HD12	1:A:2187:LEU:HD22	1.91	0.51
1:B:2321:PHE:HB2	1:B:2322:PRO:HD2	1.93	0.51
1:A:2221:ASN:ND2	1:A:2230:TYR:OH	2.44	0.51
1:B:2208:THR:HA	1:B:2212:PHE:CD1	2.45	0.51
1:B:2313:SER:HB2	1:B:2316:HIS:HB2	1.93	0.51
3:F:9:DC:H2'	3:F:10:DA:H8	1.75	0.51
1:A:2220:LEU:HA	1:A:2227:GLU:HA	1.92	0.51
1:B:1943:ASP:OD1	1:B:1943:ASP:N	2.43	0.51
1:A:1983:GLU:HA	1:A:1986:TYR:OH	2.12	0.51
1:A:2193:LEU:HG	1:A:2196:LEU:HD13	1.91	0.51
1:A:2251:ASN:HA	3:F:12:DT:H1'	1.93	0.51
1:B:2536:LEU:HD22	1:B:2543:LEU:HD12	1.93	0.50
1:B:2315:ARG:HB2	1:B:2582:TRP:CD1	2.46	0.50
1:B:1901:VAL:HG23	1:B:1902:GLY:H	1.74	0.50
1:B:2221:ASN:HB3	1:B:2224:LEU:HD13	1.93	0.50
1:A:2482:LYS:O	1:A:2485:THR:OG1	2.23	0.50
1:A:1902:GLY:HA2	1:A:1917:LEU:HD13	1.93	0.50
1:B:2216:ARG:HH21	1:B:2217:GLU:HB3	1.75	0.50
1:A:1972:LYS:HD3	1:A:2088:GLU:OE1	2.12	0.49
1:A:2087:LEU:HB2	1:A:2534:PHE:CD2	2.48	0.49
1:A:1983:GLU:O	1:A:1984:GLN:HG3	2.12	0.49
1:A:2135:GLU:O	1:A:2139:LEU:HB2	2.13	0.49
1:A:2444:LEU:HD21	1:A:2483:ILE:HD11	1.95	0.49
1:A:2442:THR:HG21	1:A:2446:ARG:HH21	1.78	0.49
1:B:2186:LYS:HE3	1:B:2190:LEU:HD23	1.95	0.49
6:A:2604:DG3:O4'	3:F:13:DG:H2'	2.12	0.49
1:A:2461:LYS:O	1:A:2465:GLU:HG3	2.13	0.49
1:B:2576:VAL:O	1:B:2586:LYS:HG3	2.13	0.49
1:B:2575:LYS:HE3	1:B:2586:LYS:HE2	1.93	0.49
1:A:1991:VAL:HG21	1:A:2081:GLN:HG3	1.95	0.48
1:B:2135:GLU:O	1:B:2139:LEU:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1844:TRP:CZ3	1:A:1951:CYS:HB3	2.48	0.48
1:A:2187:LEU:HD11	1:A:2198:LEU:HD22	1.95	0.48
1:B:2463:HIS:O	1:B:2467:GLN:HB2	2.12	0.48
1:A:2536:LEU:HD22	1:A:2543:LEU:HD12	1.94	0.48
1:B:1844:TRP:CZ3	1:B:1951:CYS:HB3	2.49	0.48
1:B:2340:ALA:HB1	1:B:2349:ILE:HD13	1.94	0.48
1:A:2232:VAL:O	1:A:2244:PHE:HA	2.14	0.48
1:B:2203:ILE:O	1:B:2207:ILE:HG22	2.12	0.48
6:B:2604:DG3:O4'	3:H:13:DG:H2'	2.14	0.48
1:A:2213:PRO:O	1:A:2217:GLU:HG2	2.14	0.48
1:A:2576:VAL:O	1:A:2586:LYS:HG3	2.13	0.48
1:B:1956:SER:C	1:B:1958:LYS:H	2.17	0.48
1:B:2427:MET:SD	4:B:2601:GOL:O1	2.66	0.48
1:A:2372:GLU:HG3	1:A:2373:SER:H	1.78	0.48
1:B:2208:THR:HA	1:B:2212:PHE:HD1	1.77	0.48
1:A:1941:LEU:HA	1:A:1944:ARG:NH1	2.29	0.48
1:B:2441:GLN:HE21	1:B:2445:GLY:HA2	1.79	0.48
1:B:2499:PHE:HZ	1:B:2505:ARG:HE	1.52	0.47
1:A:2105:ILE:HD13	1:A:2310:PHE:CE2	2.48	0.47
1:A:2427:MET:SD	4:A:2601:GOL:O1	2.72	0.47
1:A:2575:LYS:HE3	1:A:2586:LYS:HE2	1.96	0.47
1:A:2047:SER:O	1:A:2051:ILE:HG22	2.13	0.47
1:A:2534:PHE:HA	1:A:2544:TYR:CD1	2.50	0.47
1:B:2180:SER:O	1:B:2183:VAL:HG12	2.14	0.47
1:A:2084:LEU:HB3	1:A:2233:SER:HB2	1.97	0.47
1:B:2470:ASN:ND2	2:G:5:DC:H2''	2.30	0.47
1:A:2195:GLY:O	1:A:2198:LEU:HB3	2.14	0.47
1:B:2243:THR:HA	1:B:2250:GLN:HE22	1.78	0.47
1:A:2074:ARG:HG3	1:A:2075:LYS:HG2	1.96	0.47
1:B:2534:PHE:HA	1:B:2544:TYR:CD1	2.50	0.47
1:B:1837:PHE:O	1:B:1840:PHE:HB3	2.15	0.47
1:B:2234:GLN:HG3	1:B:2235:SER:O	2.13	0.47
1:A:2215:GLN:HA	1:A:2218:LYS:HE3	1.95	0.47
1:B:2184:LEU:HD12	1:B:2187:LEU:HD22	1.95	0.47
1:B:2184:LEU:O	1:B:2187:LEU:HB3	2.15	0.46
1:B:2577:LYS:HG2	1:B:2586:LYS:HB2	1.97	0.46
1:A:2481:VAL:HG21	1:A:2539:HIS:O	2.14	0.46
2:G:12:DA:H2''	2:G:13:DG:C5'	2.45	0.46
1:B:2258:ILE:HG23	1:B:2310:PHE:HB3	1.97	0.46
1:B:2374:VAL:HG13	1:B:2378:LEU:HD23	1.96	0.46
1:A:2366:TRP:HZ2	1:A:2402:MET:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2203:ILE:O	1:A:2207:ILE:HG22	2.16	0.46
1:A:2092:ILE:HB	1:A:2535:ILE:HG23	1.97	0.46
1:B:2242:ILE:HD11	1:B:2482:LYS:HE2	1.98	0.46
1:A:2499:PHE:HZ	1:A:2505:ARG:HH21	1.64	0.46
1:B:2090:ASN:ND2	1:B:2533:PHE:HB3	2.31	0.46
1:B:1852:ILE:HG12	1:B:1905:VAL:HG22	1.97	0.45
1:A:2487:ASN:HB3	1:A:2561:GLU:OE1	2.16	0.45
1:A:1941:LEU:O	1:A:1944:ARG:NH2	2.49	0.45
1:A:1956:SER:C	1:A:1958:LYS:H	2.19	0.45
1:B:2484:ALA:O	1:B:2488:ILE:HG13	2.15	0.45
1:A:2109:LYS:HB2	1:A:2258:ILE:HD11	1.98	0.45
1:B:2542:LEU:HD23	1:B:2542:LEU:HA	1.70	0.45
1:B:2030:GLN:O	1:B:2045:ARG:NH1	2.42	0.45
1:A:2481:VAL:O	1:A:2485:THR:HG23	2.16	0.45
3:H:11:DT:H4'	3:H:12:DT:OP1	2.16	0.45
1:A:2180:SER:O	1:A:2183:VAL:HG12	2.17	0.45
1:B:1968:ILE:HG13	1:B:1969:GLN:N	2.32	0.45
1:A:2470:ASN:ND2	2:E:5:DC:H2''	2.32	0.45
6:B:2604:DG3:O1G	6:B:2604:DG3:O1A	2.34	0.45
1:A:2374:VAL:HG13	1:A:2378:LEU:HD23	1.98	0.45
1:A:2392:GLY:HA3	4:A:2601:GOL:H2	1.99	0.44
1:B:1988:ASP:OD2	1:B:1990:LYS:HG2	2.17	0.44
1:B:2113:ILE:HG23	1:B:2196:LEU:HG	1.99	0.44
1:B:2125:PHE:CZ	1:B:2136:VAL:HB	2.52	0.44
1:B:2141:LEU:HD22	1:B:2186:LYS:HZ1	1.81	0.44
1:A:1968:ILE:HD11	4:A:2602:GOL:O2	2.18	0.44
1:B:2427:MET:O	1:B:2430:THR:HG22	2.17	0.44
1:B:2084:LEU:HD13	1:B:2233:SER:OG	2.18	0.44
1:B:1983:GLU:HA	1:B:1986:TYR:OH	2.17	0.44
1:B:2500:LYS:HB3	1:B:2504:HIS:CE1	2.52	0.44
1:B:2543:LEU:HD11	1:B:2582:TRP:CZ2	2.53	0.44
1:A:2234:GLN:HG3	1:A:2235:SER:O	2.17	0.44
1:B:2333:GLN:HB3	1:B:2336:LEU:HD12	1.99	0.44
1:A:1828:ILE:HD12	1:A:1913:TYR:CE1	2.52	0.44
1:A:1968:ILE:HG13	1:A:1969:GLN:N	2.32	0.44
1:A:2397:SER:O	1:A:2400:GLU:HB3	2.18	0.44
1:A:2498:THR:OG1	1:A:2499:PHE:N	2.51	0.44
1:A:2500:LYS:HE2	1:A:2500:LYS:HB2	1.80	0.44
1:B:2220:LEU:HD12	1:B:2222:PRO:HD3	2.00	0.44
1:B:2366:TRP:HZ2	1:B:2402:MET:HB3	1.82	0.44
2:G:1:DC:H3'	2:G:2:DG:H5''	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1975:LEU:HD23	1:A:2089:LEU:HD13	1.99	0.44
1:A:2184:LEU:O	1:A:2187:LEU:HB3	2.16	0.44
1:B:2324:GLY:HA2	1:B:2547:ALA:HA	1.99	0.44
1:A:2238:ALA:HB1	1:A:2448:ARG:CZ	2.47	0.44
1:A:2254:ARG:HD3	1:A:2376:ASP:OD2	2.17	0.44
1:B:2384:GLN:HB2	1:B:2384:GLN:HE21	1.58	0.43
1:B:2102:GLN:HA	1:B:2105:ILE:HD12	1.99	0.43
3:F:11:DT:H4'	3:F:12:DT:OP1	2.18	0.43
1:A:1825:LEU:HD11	1:A:1827:ILE:HG12	2.00	0.43
1:A:2125:PHE:CZ	1:A:2136:VAL:HB	2.54	0.43
1:B:1855:ALA:HB1	1:B:2045:ARG:NH2	2.33	0.43
1:B:2340:ALA:HB1	1:B:2349:ILE:CD1	2.47	0.43
1:B:2341:HIS:HD2	1:B:2342:LEU:HD12	1.83	0.43
1:A:2241:ARG:HH12	3:F:13:DG:H21	1.65	0.43
1:B:2072:VAL:O	1:B:2076:VAL:HB	2.17	0.43
1:B:1994:TRP:CZ2	1:B:2240:GLY:HA2	2.53	0.43
1:A:2217:GLU:HG3	1:A:2229:ILE:HD11	2.01	0.43
1:B:1940:THR:HB	1:B:1943:ASP:HB2	2.00	0.43
1:B:2256:PHE:CZ	1:B:2312:ILE:HD11	2.54	0.43
2:E:8:DT:H3	3:F:10:DA:H61	1.65	0.43
1:A:1855:ALA:HB1	1:A:2045:ARG:NH2	2.34	0.43
1:A:2500:LYS:HB3	1:A:2504:HIS:CE1	2.53	0.43
1:B:2500:LYS:HB2	1:B:2500:LYS:HE2	1.85	0.43
1:B:2538:LEU:HB2	1:B:2541:GLU:HB3	2.00	0.43
3:F:11:DT:H2'	3:F:12:DT:C6	2.53	0.43
1:B:1969:GLN:HA	1:B:1972:LYS:HB2	2.00	0.43
1:A:2542:LEU:HD23	1:A:2542:LEU:HA	1.80	0.43
3:F:12:DT:H6	3:F:12:DT:H5''	1.83	0.43
1:A:2102:GLN:HA	1:A:2105:ILE:HD12	2.01	0.42
1:A:2113:ILE:HD13	1:A:2113:ILE:HA	1.88	0.42
1:A:2249:ILE:HA	1:A:2252:VAL:HG13	2.00	0.42
1:B:2330:ASP:OD1	1:B:2331:TYR:O	2.37	0.42
1:B:2482:LYS:O	1:B:2485:THR:OG1	2.29	0.42
1:A:1897:ASP:N	1:A:1897:ASP:OD1	2.53	0.42
1:A:2023:MET:CE	1:A:2048:VAL:HG11	2.50	0.42
1:B:1849:ARG:NH1	1:B:1987:GLU:OE1	2.50	0.42
1:B:2255:ASP:N	1:B:2255:ASP:OD1	2.52	0.42
1:A:2340:ALA:HB1	1:A:2349:ILE:HD13	2.00	0.42
1:B:2084:LEU:HD21	1:B:2242:ILE:HG21	2.00	0.42
1:A:1994:TRP:HB2	1:A:2236:HIS:NE2	2.34	0.42
1:B:1991:VAL:HG21	1:B:2081:GLN:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2191:HIS:O	1:B:2193:LEU:N	2.51	0.42
1:B:2536:LEU:HD23	1:B:2537:GLN:N	2.34	0.42
1:A:2130:SER:HA	1:A:2133:ILE:HD12	2.00	0.42
1:A:2427:MET:O	1:A:2430:THR:HG22	2.19	0.42
1:A:2536:LEU:HD23	1:A:2537:GLN:N	2.35	0.42
1:B:2238:ALA:HB1	1:B:2448:ARG:CZ	2.50	0.42
1:A:2415:SER:O	1:A:2419:ARG:HG2	2.20	0.42
1:A:2384:GLN:HB2	1:A:2384:GLN:HE21	1.64	0.42
1:A:2583:GLY:C	1:A:2584:GLU:HG3	2.40	0.42
1:B:1897:ASP:OD1	1:B:1897:ASP:N	2.50	0.42
1:A:1837:PHE:O	1:A:1840:PHE:HB3	2.20	0.42
1:A:1969:GLN:HA	1:A:1972:LYS:HB2	2.02	0.42
1:A:2470:ASN:ND2	2:E:6:DA:H5'	2.30	0.42
1:A:1964:ILE:O	1:A:1989:PRO:HD2	2.19	0.41
1:A:2204:THR:O	1:A:2208:THR:HG22	2.20	0.41
1:A:2256:PHE:CZ	1:A:2312:ILE:HD11	2.55	0.41
1:A:1975:LEU:O	1:A:1979:GLY:HA2	2.20	0.41
1:A:1988:ASP:OD2	1:A:1990:LYS:HG2	2.20	0.41
1:B:1825:LEU:HD11	1:B:1827:ILE:HG12	2.02	0.41
1:B:1956:SER:O	1:B:1958:LYS:N	2.53	0.41
1:B:1994:TRP:HB2	1:B:2236:HIS:NE2	2.35	0.41
1:B:2505:ARG:O	1:B:2508:MET:HB3	2.20	0.41
1:B:2583:GLY:C	1:B:2584:GLU:HG3	2.40	0.41
1:A:1956:SER:O	1:A:1958:LYS:N	2.53	0.41
1:A:2412:TYR:O	1:A:2415:SER:HB3	2.21	0.41
1:A:2484:ALA:O	1:A:2488:ILE:HG13	2.20	0.41
1:B:1964:ILE:O	1:B:1989:PRO:HD2	2.20	0.41
1:A:1828:ILE:HD12	1:A:1913:TYR:HE1	1.84	0.41
1:B:2105:ILE:HD13	1:B:2310:PHE:CE2	2.56	0.41
2:E:12:DA:H2''	2:E:13:DG:C5'	2.51	0.41
1:B:1968:ILE:O	1:B:1972:LYS:HG3	2.20	0.41
1:B:2249:ILE:HA	1:B:2252:VAL:HG13	2.02	0.41
1:A:2237:THR:OG1	1:A:2241:ARG:N	2.54	0.41
1:A:1940:THR:HB	1:A:1943:ASP:HB2	2.02	0.41
1:A:2457:ASN:HA	1:A:2458:PRO:HD3	1.85	0.41
2:G:1:DC:H2'	2:G:2:DG:N7	2.36	0.41
1:A:2543:LEU:HA	1:A:2543:LEU:HD23	1.76	0.41
2:G:4:DC:H2''	2:G:5:DC:H5'	2.02	0.41
2:G:5:DC:H2''	2:G:6:DA:H5'	2.02	0.41
1:A:2433:ASN:O	1:A:2436:ARG:HG2	2.20	0.41
1:B:2180:SER:HB2	3:H:10:DA:OP2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2141:LEU:HD13	1:B:2186:LYS:HZ1	1.86	0.41
1:A:2443:ILE:HG13	1:A:2476:SER:OG	2.21	0.40
1:B:1952:LEU:HD23	1:B:1982:LEU:HD13	2.02	0.40
1:B:1988:ASP:HA	1:B:1989:PRO:HD2	1.93	0.40
1:B:2204:THR:O	1:B:2208:THR:HG22	2.21	0.40
1:B:1975:LEU:O	1:B:1979:GLY:HA2	2.21	0.40
1:A:1859:ILE:HG23	1:A:1859:ILE:O	2.21	0.40
1:B:2186:LYS:HB3	1:B:2194:PRO:HB3	2.03	0.40
1:B:2443:ILE:HG13	1:B:2476:SER:OG	2.22	0.40
1:B:1941:LEU:HA	1:B:1944:ARG:NH1	2.36	0.40
1:B:2049:GLU:HG2	1:B:2053:ILE:HD12	2.04	0.40
2:G:5:DC:H2'	2:G:6:DA:C8	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	613/772 (79%)	545 (89%)	67 (11%)	1 (0%)	49	83
1	B	613/772 (79%)	541 (88%)	70 (11%)	2 (0%)	43	79
All	All	1226/1544 (79%)	1086 (89%)	137 (11%)	3 (0%)	49	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2144	PRO
1	B	2144	PRO
1	B	1859	ILE

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	551/675 (82%)	533 (97%)	18 (3%)	41	70
1	B	551/675 (82%)	532 (97%)	19 (3%)	40	69
All	All	1102/1350 (82%)	1065 (97%)	37 (3%)	40	69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1854	LEU
1	A	1858	LYS
1	A	1899	LEU
1	A	1943	ASP
1	A	2141	LEU
1	A	2177	PHE
1	A	2187	LEU
1	A	2236	HIS
1	A	2245	THR
1	A	2377	ASP
1	A	2384	GLN
1	A	2393	MET
1	A	2416	PHE
1	A	2424	ASN
1	A	2470	ASN
1	A	2537	GLN
1	A	2566	VAL
1	A	2582	TRP
1	B	1854	LEU
1	B	1858	LYS
1	B	1899	LEU
1	B	1943	ASP
1	B	1977	SER
1	B	2141	LEU
1	B	2177	PHE
1	B	2236	HIS
1	B	2245	THR

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Mol	Chain	Res	Type
1	B	2255	ASP
1	B	2377	ASP
1	B	2384	GLN
1	B	2393	MET
1	B	2416	PHE
1	B	2424	ASN
1	B	2470	ASN
1	B	2537	GLN
1	B	2566	VAL
1	B	2582	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1838	GLN
1	A	1984	GLN
1	A	2061	ASN
1	A	2215	GLN
1	A	2221	ASN
1	A	2384	GLN
1	A	2470	ASN
1	B	1984	GLN
1	B	2215	GLN
1	B	2384	GLN
1	B	2470	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 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	2601	-	5,5,5	0.33	0	5,5,5	0.32	0
4	GOL	A	2602	-	5,5,5	0.39	0	5,5,5	0.35	0
6	DG3	A	2604	5	26,32,32	1.17	2 (7%)	26,50,50	2.75	10 (38%)
4	GOL	B	2601	-	5,5,5	0.35	0	5,5,5	0.32	0
4	GOL	B	2602	-	5,5,5	0.38	0	5,5,5	0.46	0
6	DG3	B	2604	5	26,32,32	1.18	2 (7%)	26,50,50	2.67	11 (42%)

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
4	GOL	A	2601	-	-	0/4/4/4	0/0/0/0
4	GOL	A	2602	-	-	0/4/4/4	0/0/0/0
6	DG3	A	2604	5	-	0/18/31/31	0/3/3/3
4	GOL	B	2601	-	-	0/4/4/4	0/0/0/0
4	GOL	B	2602	-	-	0/4/4/4	0/0/0/0
6	DG3	B	2604	5	-	0/18/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2604	DG3	C5-C4	2.99	1.47	1.40
6	B	2604	DG3	C5-C4	3.06	1.47	1.40
6	A	2604	DG3	C6-C5	4.14	1.48	1.41
6	B	2604	DG3	C6-C5	4.22	1.48	1.41

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2604	DG3	PA-O3A-PB	-5.89	112.83	132.63
6	B	2604	DG3	PA-O3A-PB	-5.64	113.69	132.63
6	A	2604	DG3	PB-O3B-PG	-5.23	115.03	132.63
6	B	2604	DG3	PB-O3B-PG	-5.09	115.52	132.63
6	A	2604	DG3	C6-C5-C4	-4.20	116.72	120.85
6	B	2604	DG3	C6-C5-C4	-4.08	116.84	120.85
6	B	2604	DG3	C5-C6-N1	-3.76	118.12	123.47
6	A	2604	DG3	C5-C6-N1	-3.71	118.19	123.47
6	A	2604	DG3	N3-C2-N1	-3.25	122.65	127.41
6	B	2604	DG3	N3-C2-N1	-3.07	122.91	127.41
6	B	2604	DG3	C4-C5-N7	-3.05	106.46	109.41
6	A	2604	DG3	C4-C5-N7	-2.91	106.60	109.41
6	B	2604	DG3	O4'-C1'-N9	2.02	111.19	107.78
6	A	2604	DG3	O3G-PG-O2G	2.07	115.78	107.59
6	B	2604	DG3	O3G-PG-O2G	2.22	116.38	107.59
6	B	2604	DG3	C3'-C2'-C1'	2.67	106.01	102.80
6	A	2604	DG3	C3'-C2'-C1'	2.93	106.32	102.80
6	B	2604	DG3	C6-N1-C2	4.23	122.14	116.06
6	A	2604	DG3	C6-N1-C2	4.24	122.16	116.06
6	B	2604	DG3	C2-N3-C4	5.01	121.01	115.16
6	A	2604	DG3	C2-N3-C4	5.16	121.19	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2601	GOL	2	0
4	A	2602	GOL	1	0
6	A	2604	DG3	4	0
4	B	2601	GOL	1	0
6	B	2604	DG3	4	0

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	625/772 (80%)	0.18	28 (4%) 33 26	72, 137, 251, 323	0
1	B	625/772 (80%)	0.18	40 (6%) 19 14	65, 128, 234, 303	0
2	E	13/17 (76%)	0.86	1 (7%) 13 10	118, 139, 269, 363	0
2	G	13/17 (76%)	0.50	1 (7%) 13 10	98, 130, 231, 307	0
3	F	9/13 (69%)	0.24	0 100 100	115, 135, 286, 323	0
3	H	9/13 (69%)	0.23	1 (11%) 5 5	110, 134, 214, 256	0
All	All	1294/1604 (80%)	0.19	71 (5%) 25 20	65, 132, 242, 363	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2178	SER	8.4
1	B	2307	GLY	7.7
1	A	2179	THR	7.4
1	A	2307	GLY	6.7
1	B	2135	GLU	5.8
1	B	2120	LEU	4.9
1	A	2587	ASP	4.8
2	E	13	DG	4.2
1	A	2135	GLU	4.2
1	B	2117	ALA	4.1
1	A	2185	ASN	4.0
1	B	2015	HIS	4.0
1	A	2177	PHE	3.9
1	A	2117	ALA	3.8
1	A	2137	LEU	3.8
1	A	2176	GLN	3.7
1	B	1833	ASP	3.6
1	B	2133	ILE	3.6
1	B	2587	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	2178	SER	3.4
1	A	2139	LEU	3.4
1	B	1936	ASP	3.3
1	B	2193	LEU	3.1
1	B	2185	ASN	3.1
1	B	2589	ASP	3.1
1	B	2141	LEU	3.1
1	A	2182	ASP	3.1
1	A	2141	LEU	3.0
1	B	2402	MET	3.0
1	A	2590	VAL	3.0
1	B	1835	ASN	3.0
1	B	2188	LYS	3.0
1	A	2027	GLN	3.0
1	B	2137	LEU	3.0
1	A	2454	LYS	3.0
1	B	2189	ALA	2.9
1	B	2035	ASN	2.9
1	B	2179	THR	2.9
1	B	2546	VAL	2.8
1	A	2028	GLY	2.7
1	A	2138	PHE	2.7
1	B	1957	ASP	2.7
1	A	2589	ASP	2.7
2	G	13	DG	2.6
1	A	1935	LEU	2.5
3	H	13	DG	2.5
1	B	2134	ALA	2.5
1	A	2012	PHE	2.5
1	A	2402	MET	2.5
1	B	2113	ILE	2.5
1	B	2590	VAL	2.4
1	B	2044	TYR	2.4
1	B	2588	PHE	2.4
1	B	1965	TYR	2.3
1	B	2139	LEU	2.3
1	B	2531	GLY	2.3
1	A	2308	MET	2.3
1	B	2553	GLN	2.3
1	A	2133	ILE	2.2
1	B	2455	ASP	2.2
1	A	2188	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	2015	HIS	2.2
1	B	2194	PRO	2.2
1	B	2309	PRO	2.2
1	B	2452	GLY	2.2
1	B	2177	PHE	2.2
1	B	2454	LYS	2.1
1	A	2123	HIS	2.1
1	B	2192	PRO	2.0
1	A	1833	ASP	2.0
1	B	1834	GLN	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(Å ²)	Q<0.9
4	GOL	A	2601	6/6	0.60	0.61	120,136,145,151	0
4	GOL	B	2601	6/6	0.62	0.58	107,137,143,147	0
4	GOL	B	2602	6/6	0.88	0.38	54,55,56,56	0
5	MG	B	2603	1/1	0.91	0.27	76,76,76,76	0
4	GOL	A	2602	6/6	0.91	0.46	72,72,73,79	0
6	DG3	B	2604	30/30	0.92	0.32	72,76,113,120	0
6	DG3	A	2604	30/30	0.92	0.33	95,102,141,146	0
5	MG	A	2603	1/1	0.93	0.31	95,95,95,95	0

6.5 Other polymers [i](#)

There are no such residues in this entry.