Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 04:11 pm GMT

PDB ID	:	2W9C
Title	:	Ternary complex of Dpo4 bound to N2,N2-dimethyl-deoxyguanosine modified DNA with incoming dTTP
Authors	:	Eoff, R.L.; Zhang, H.; Kosekov, I.D.; Rizzo, C.J.; Egli, M.; Guengerich, F.P.
Deposited on	:	2009-01-22
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

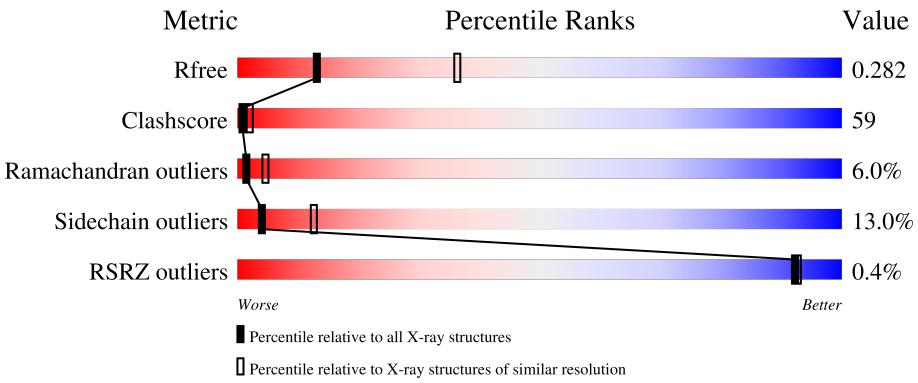
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	28% 56% 11% • •
2	B	358	% 24% 59% 12% • •
3	C	13	23% 77%
3	D	13	15% 77% 8%
4	E	18	33% 44% 11% 11%

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Mol	Chain	Length	Quality of chain
4	F	18	6% 61% 22% 11%

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	O2G	E	5	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6843 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 IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	342	2746	1760	475	504	7	0	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	ARG	LYS	conflict	UNP Q97W02

- Molecule 2 is a protein called DNA POLYMERASE IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	342	2744	1760	473	504	7	0	0	1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	272	129	57	74	12	0	0	0
3	D	13	272	129	57	74	12	0	0	0

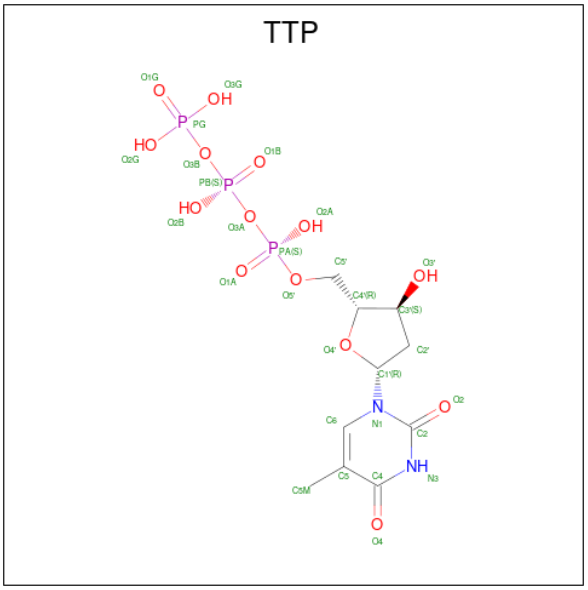
- Molecule 4 is a DNA chain called 5'-D(*TP*CP*AP*CP*O2GP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	E	16	318	154	55	94	15	0	0	0
4	F	16	318	154	55	94	15	0	0	0

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

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

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C N O P 29 10 2 14 3	0	0
6	B	1	Total C N O P 29 10 2 14 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	43	Total O 43 43	0	0
7	B	40	Total O 40 40	0	0
7	C	9	Total O 9 9	0	0
7	D	6	Total O 6 6	0	0

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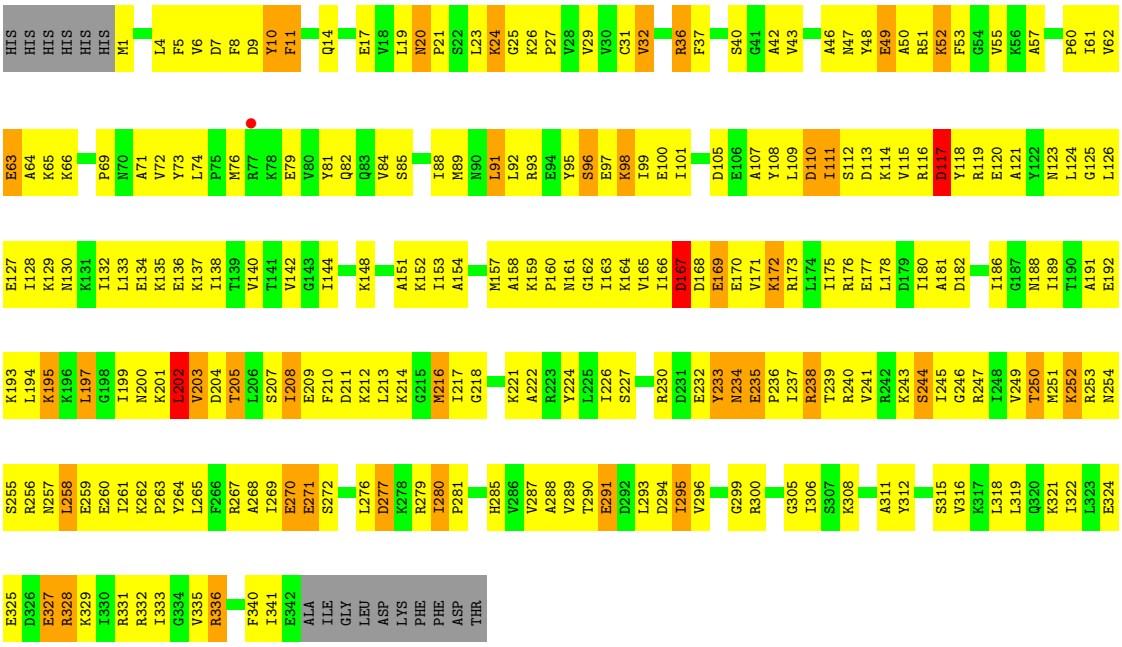
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	E	5	5	5	0	0
			Total	O		
7	F	6	6	6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

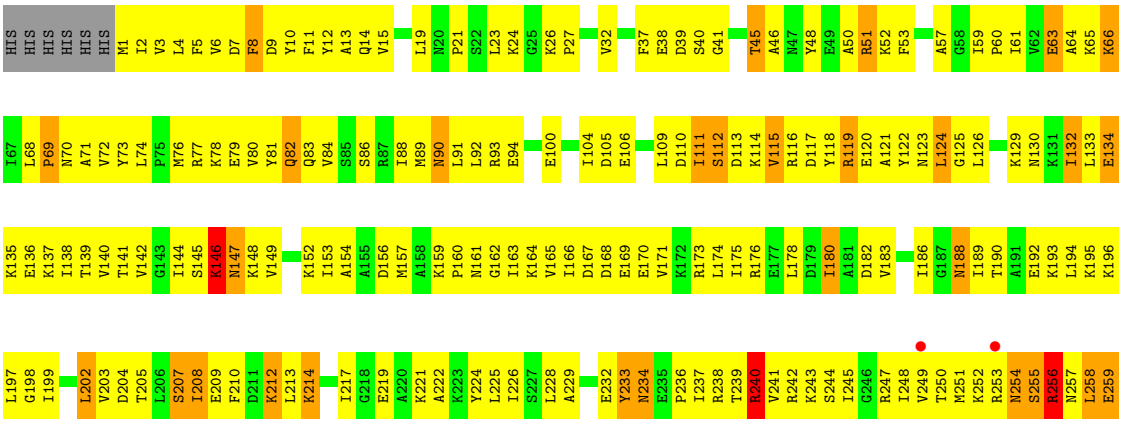
• Molecule 1: DNA POLYMERASE IV

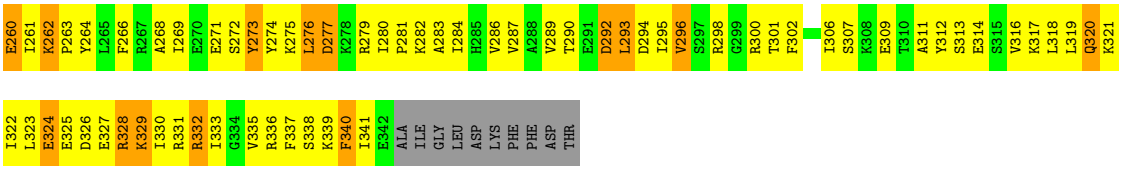
Chain A: 28% 56% 11%



• Molecule 2: DNA POLYMERASE IV

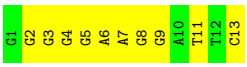
Chain B: % 24% 59% 12%





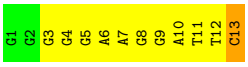
• Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*DOCP)-3'

Chain C:



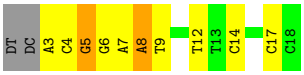
• Molecule 3: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP *TP*TP*DOCP)-3'

Chain D:



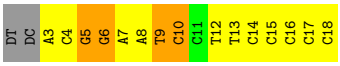
• Molecule 4: 5'-D(*TP*CP*AP*CP*O2GP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*C)-3'

Chain E:



• Molecule 4: 5'-D(*TP*CP*AP*CP*O2GP*GP*AP*AP*TP*CP*CP *TP*TP*CP*CP*CP*CP*C)-3'

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	51.71Å 101.62Å 96.75Å 90.00° 92.29° 90.00°	Depositor
Resolution (Å)	28.33 – 2.90 28.33 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.33-2.90) 86.9 (28.33-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.90Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.252 , 0.288 0.247 , 0.282	Depositor DCC
R_{free} test set	1055 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.169 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	6843	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, O2G, DOC, TTP

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	0.46	0/2785	0.72	0/3741
2	B	0.47	0/2783	0.74	2/3738 (0.1%)
3	C	0.48	0/287	0.69	0/444
3	D	0.47	0/287	0.69	0/444
4	E	0.62	0/326	0.83	0/496
4	F	0.69	0/326	1.01	0/496
All	All	0.49	0/6794	0.75	2/9359 (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
4	E	0	1
4	F	0	3
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	256	ARG	NE-CZ-NH2	8.25	124.43	120.30
2	B	256	ARG	NE-CZ-NH1	-7.18	116.71	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	E	8	DA	Sidechain
4	F	10	DC	Sidechain
4	F	6	DG	Sidechain
4	F	9	DT	Sidechain

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	2746	0	2889	371	1
2	B	2744	0	2889	351	0
3	C	272	0	146	17	0
3	D	272	0	146	16	0
4	E	318	0	185	33	0
4	F	318	0	185	27	1
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	29	0	13	5	0
6	B	29	0	13	4	0
7	A	43	0	0	15	0
7	B	40	0	0	16	0
7	C	9	0	0	1	0
7	D	6	0	0	3	0
7	E	5	0	0	0	0
7	F	6	0	0	5	0
All	All	6843	0	6466	783	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 59.

All (783) 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)
2:B:258:LEU:CD1	2:B:262:LYS:HE3	1.53	1.35
2:B:258:LEU:HD11	2:B:262:LYS:CE	1.57	1.33
1:A:210:PHE:HE1	1:A:226:ILE:CD1	1.49	1.24
3:D:11:DT:H5'	7:D:2006:HOH:O	1.37	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:HH12	2:B:327:GLU:C	1.44	1.20
1:A:210:PHE:CE1	1:A:226:ILE:CD1	2.25	1.20
1:A:210:PHE:CE1	1:A:226:ILE:HD13	1.79	1.15
2:B:258:LEU:CD1	2:B:259:GLU:N	2.11	1.13
2:B:256:ARG:HH12	2:B:328:ARG:N	1.47	1.10
1:A:208:ILE:HD11	1:A:212:LYS:HG2	1.13	1.09
1:A:256:ARG:NH2	1:A:327:GLU:HA	1.69	1.08
1:A:133:LEU:HD22	7:A:2026:HOH:O	1.50	1.08
3:C:4:DG:H2"	3:C:5:DG:H5"	1.35	1.07
2:B:4:LEU:HB2	2:B:111:ILE:HD11	1.34	1.07
1:A:208:ILE:HD13	1:A:209:GLU:H	1.13	1.06
1:A:100:GLU:HB3	1:A:108:TYR:HB2	1.35	1.06
2:B:329:LYS:H	2:B:329:LYS:HD2	1.15	1.05
2:B:258:LEU:HD13	2:B:259:GLU:N	1.72	1.04
1:A:210:PHE:HE1	1:A:226:ILE:HD13	0.86	1.02
2:B:146:LYS:HB2	2:B:146:LYS:NZ	1.74	1.02
2:B:105:ASP:HB2	7:B:2036:HOH:O	1.57	1.02
1:A:199:ILE:HG23	7:A:2035:HOH:O	1.59	1.01
2:B:148:LYS:HD3	2:B:237:ILE:HG12	1.42	0.99
2:B:100:GLU:OE2	2:B:148:LYS:HE2	1.61	0.99
2:B:195:LYS:HA	7:B:2027:HOH:O	1.63	0.98
1:A:256:ARG:HH21	1:A:327:GLU:HA	1.28	0.97
1:A:208:ILE:HD11	1:A:212:LYS:CG	1.94	0.97
1:A:256:ARG:HG2	1:A:256:ARG:HH11	1.26	0.96
2:B:262:LYS:HE2	2:B:316:VAL:HG13	1.48	0.96
2:B:146:LYS:HB2	2:B:146:LYS:HZ2	1.27	0.95
1:A:208:ILE:CD1	1:A:209:GLU:H	1.80	0.95
1:A:204:ASP:HB2	7:A:2035:HOH:O	1.66	0.94
2:B:110:ASP:HB2	2:B:237:ILE:HD12	1.47	0.94
1:A:210:PHE:CE1	1:A:226:ILE:HD11	2.00	0.93
2:B:258:LEU:HD12	2:B:259:GLU:N	1.82	0.93
1:A:311:ALA:O	1:A:315:SER:HB2	1.70	0.92
1:A:114:LYS:H	1:A:114:LYS:HD2	1.35	0.91
1:A:247:ARG:HD3	1:A:271:GLU:HG2	1.51	0.90
4:E:3:DA:C2'	4:E:4:DC:H5'	2.01	0.90
2:B:256:ARG:NH1	2:B:328:ARG:N	2.20	0.90
2:B:111:ILE:HD13	2:B:111:ILE:H	1.36	0.90
1:A:116:ARG:O	1:A:117:ASP:HB3	1.71	0.89
1:A:208:ILE:CD1	1:A:212:LYS:HG2	2.02	0.88
1:A:208:ILE:HD13	1:A:209:GLU:N	1.87	0.88
2:B:146:LYS:NZ	2:B:146:LYS:CB	2.35	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:LYS:H	2:B:329:LYS:CD	1.80	0.88
2:B:256:ARG:NH1	2:B:327:GLU:C	2.26	0.88
1:A:208:ILE:CD1	1:A:209:GLU:N	2.36	0.87
6:B:1345:TTP:O1B	7:B:2038:HOH:O	1.91	0.87
1:A:32:VAL:HG13	1:A:76:MET:HE2	1.55	0.87
1:A:200:ASN:HB3	1:A:201:LYS:HZ3	1.40	0.87
2:B:12:TYR:HB2	2:B:45:THR:CG2	2.05	0.87
2:B:258:LEU:HD13	2:B:258:LEU:C	1.95	0.86
1:A:208:ILE:HD12	1:A:212:LYS:HB3	1.57	0.84
2:B:78:LYS:HA	2:B:81:TYR:CD2	2.12	0.84
2:B:282:LYS:HD2	7:B:2032:HOH:O	1.76	0.83
2:B:105:ASP:CB	7:B:2036:HOH:O	2.20	0.83
3:C:4:DG:C2'	3:C:5:DG:H5"	2.07	0.82
1:A:111:ILE:CD1	1:A:124:LEU:HD23	2.09	0.82
2:B:258:LEU:HD12	2:B:259:GLU:H	1.40	0.81
2:B:329:LYS:HD2	2:B:329:LYS:N	1.94	0.81
2:B:319:LEU:HA	2:B:322:ILE:HD12	1.62	0.81
2:B:4:LEU:HB2	2:B:111:ILE:CD1	2.11	0.81
1:A:178:LEU:HD11	1:A:182:ASP:HB2	1.62	0.81
4:F:18:DC:O4'	7:F:2006:HOH:O	1.98	0.80
1:A:98:LYS:NZ	1:A:110:ASP:HB3	1.96	0.80
1:A:170:GLU:HG3	1:A:173:ARG:NH2	1.97	0.80
1:A:331:ARG:HH12	4:E:5:O2G:P	2.04	0.80
2:B:12:TYR:HB2	2:B:45:THR:HG21	1.64	0.80
1:A:31:CYS:HB3	1:A:43:VAL:HA	1.62	0.80
2:B:298:ARG:HB3	2:B:318:LEU:HD22	1.63	0.80
1:A:235:GLU:HG2	1:A:236:PRO:HD2	1.64	0.80
2:B:116:ARG:O	2:B:117:ASP:HB3	1.82	0.79
4:E:3:DA:H2"	4:E:4:DC:H5'	1.65	0.79
2:B:194:LEU:HD21	2:B:217:ILE:HD13	1.64	0.79
2:B:326:ASP:CG	2:B:327:GLU:H	1.85	0.78
2:B:114:LYS:O	2:B:115:VAL:HB	1.83	0.78
1:A:193:LYS:HB3	1:A:216:MET:CG	2.13	0.78
4:F:16:DC:H2'	4:F:17:DC:C6	2.17	0.78
1:A:180:ILE:HB	1:A:200:ASN:O	1.83	0.78
1:A:321:LYS:HE2	1:A:325:GLU:OE1	1.84	0.78
1:A:36:ARG:NH2	1:A:331:ARG:HG3	1.99	0.78
2:B:19:LEU:HD23	2:B:77:ARG:HH22	1.48	0.78
2:B:262:LYS:HE2	2:B:316:VAL:CG1	2.14	0.78
2:B:180:ILE:HD13	2:B:180:ILE:O	1.84	0.77
1:A:222:ALA:O	1:A:226:ILE:HD12	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:46:ALA:O	2:B:51:ARG:HD2	1.85	0.77
2:B:282:LYS:HB2	2:B:339:LYS:O	1.84	0.77
1:A:109:LEU:O	1:A:237:ILE:HG12	1.83	0.76
2:B:146:LYS:CB	2:B:146:LYS:HZ3	1.98	0.76
1:A:9:ASP:HA	7:A:2043:HOH:O	1.85	0.76
1:A:173:ARG:O	1:A:177:GLU:HG2	1.85	0.76
2:B:111:ILE:HD13	2:B:111:ILE:N	1.99	0.76
1:A:96:SER:HB3	1:A:109:LEU:CD2	2.16	0.76
2:B:209:GLU:HB2	2:B:212:LYS:HB2	1.69	0.75
2:B:167:ASP:O	2:B:171:VAL:HG23	1.86	0.75
2:B:213:LEU:HD22	2:B:217:ILE:HD11	1.67	0.75
1:A:208:ILE:HD12	1:A:212:LYS:CB	2.16	0.75
2:B:318:LEU:O	2:B:322:ILE:HG13	1.87	0.75
2:B:3:VAL:HG22	2:B:237:ILE:HD11	1.68	0.74
1:A:60:PRO:HB3	4:E:3:DA:H2"	1.68	0.74
1:A:200:ASN:HB3	1:A:201:LYS:NZ	2.02	0.74
1:A:280:ILE:CG2	1:A:305:GLY:HA3	2.16	0.74
1:A:251:MET:HE1	1:A:261:ILE:HG12	1.67	0.74
1:A:8:PHE:CD2	1:A:105:ASP:HA	2.22	0.74
1:A:295:ILE:HG12	1:A:296:VAL:N	2.02	0.74
3:C:5:DG:H2"	3:C:6:DA:C8	2.24	0.73
2:B:111:ILE:HG21	2:B:124:LEU:HD22	1.70	0.73
4:F:17:DC:H2"	7:F:2006:HOH:O	1.89	0.73
2:B:105:ASP:CG	7:B:2036:HOH:O	2.26	0.73
2:B:236:PRO:HB3	7:B:2028:HOH:O	1.89	0.72
2:B:280:ILE:O	2:B:340:PHE:HA	1.89	0.72
1:A:5:PHE:CZ	1:A:152:LYS:HD3	2.25	0.72
1:A:111:ILE:HD12	1:A:124:LEU:HD23	1.72	0.72
1:A:153:ILE:HG22	1:A:157:MET:HE2	1.71	0.72
2:B:141:THR:HG23	2:B:162:GLY:C	2.09	0.72
4:E:3:DA:H2'	4:E:4:DC:H5'	1.70	0.71
1:A:259:GLU:OE1	1:A:262:LYS:HD2	1.89	0.71
2:B:147:ASN:HB3	2:B:233:TYR:CD2	2.25	0.71
1:A:188:ASN:O	1:A:192:GLU:HG2	1.90	0.71
1:A:331:ARG:NH2	4:E:5:O2G:OP1	2.24	0.71
1:A:197:LEU:CD1	1:A:212:LYS:HG3	2.20	0.71
2:B:258:LEU:CD1	2:B:259:GLU:H	1.98	0.71
2:B:4:LEU:CB	2:B:111:ILE:HD11	2.19	0.71
2:B:60:PRO:HB3	4:F:4:DC:H5'	1.73	0.71
1:A:208:ILE:CD1	1:A:212:LYS:CB	2.68	0.71
1:A:176:ARG:NH2	7:A:2027:HOH:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:LYS:HZ3	1:A:110:ASP:HB3	1.54	0.70
3:D:5:DG:H2"	3:D:6:DA:OP2	1.91	0.70
1:A:100:GLU:N	1:A:108:TYR:O	2.24	0.70
2:B:115:VAL:HG13	2:B:120:GLU:HB3	1.73	0.70
2:B:188:ASN:O	2:B:192:GLU:HG2	1.91	0.70
2:B:10:TYR:CD1	2:B:10:TYR:O	2.44	0.70
1:A:195:LYS:HD2	1:A:199:ILE:O	1.91	0.70
2:B:236:PRO:CB	7:B:2028:HOH:O	2.39	0.70
2:B:91:LEU:HD23	2:B:91:LEU:O	1.93	0.69
1:A:336:ARG:NH1	4:E:8:DA:H2'	2.06	0.69
2:B:32:VAL:HG21	4:F:5:O2G:HM1A	1.75	0.69
2:B:110:ASP:CB	2:B:237:ILE:HD12	2.22	0.69
1:A:261:ILE:HG21	1:A:319:LEU:HD21	1.73	0.69
1:A:32:VAL:CG1	1:A:76:MET:HE2	2.22	0.69
1:A:144:ILE:HG22	1:A:165:VAL:HG23	1.74	0.69
1:A:236:PRO:HG2	1:A:238:ARG:NH1	2.07	0.69
2:B:186:ILE:HG23	2:B:190:THR:HG22	1.75	0.69
2:B:208:ILE:HG22	2:B:209:GLU:H	1.57	0.69
1:A:92:LEU:HD21	1:A:132:ILE:HD11	1.74	0.69
2:B:147:ASN:HB3	2:B:233:TYR:HD2	1.58	0.68
1:A:331:ARG:NH1	4:E:5:O2G:OP1	2.26	0.68
1:A:126:LEU:O	1:A:130:ASN:HB2	1.93	0.68
1:A:100:GLU:HB3	1:A:108:TYR:CB	2.19	0.68
2:B:38:GLU:O	2:B:39:ASP:HB2	1.93	0.68
1:A:153:ILE:O	1:A:157:MET:HG2	1.94	0.68
2:B:4:LEU:HD21	2:B:142:VAL:HG13	1.76	0.68
2:B:292:ASP:OD1	2:B:292:ASP:N	2.27	0.68
2:B:109:LEU:O	2:B:111:ILE:HD13	1.93	0.68
1:A:180:ILE:HG22	1:A:195:LYS:HE3	1.76	0.68
1:A:208:ILE:HD12	1:A:209:GLU:N	2.09	0.68
1:A:171:VAL:HG12	1:A:171:VAL:O	1.94	0.67
4:E:5:O2G:O5'	4:E:5:O2G:H8	1.93	0.67
2:B:207:SER:O	2:B:208:ILE:HD13	1.94	0.67
1:A:79:GLU:CD	1:A:79:GLU:H	1.98	0.67
1:A:291:GLU:OE1	1:A:331:ARG:HD2	1.95	0.67
2:B:37:PHE:CD2	2:B:40:SER:HB3	2.29	0.67
2:B:88:ILE:HG23	2:B:132:ILE:HD13	1.77	0.67
1:A:331:ARG:HH22	4:E:4:DC:H3'	1.60	0.66
2:B:164:LYS:HG3	2:B:165:VAL:N	2.10	0.66
2:B:256:ARG:O	2:B:256:ARG:HD3	1.95	0.66
2:B:59:ILE:HD12	2:B:63:GLU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:116:ARG:HH12	1.94	0.66
2:B:171:VAL:O	2:B:175:ILE:HG12	1.96	0.66
4:F:12:DT:OP2	7:F:2005:HOH:O	2.12	0.66
1:A:111:ILE:HD13	1:A:124:LEU:HD23	1.77	0.66
4:E:5:O2G:HM1B	4:E:6:DG:O4'	1.96	0.66
1:A:170:GLU:C	1:A:172:LYS:H	1.99	0.66
2:B:307:SER:HB2	2:B:309:GLU:OE2	1.96	0.66
3:D:4:DG:H2"	3:D:5:DG:OP2	1.96	0.66
1:A:177:GLU:O	1:A:201:LYS:HD2	1.96	0.66
1:A:29:VAL:HG21	1:A:73:TYR:CE2	2.31	0.66
2:B:269:ILE:HG13	2:B:335:VAL:HG11	1.78	0.66
1:A:252:LYS:HE3	1:A:252:LYS:HA	1.76	0.65
1:A:256:ARG:HH11	1:A:256:ARG:CG	2.04	0.65
1:A:20:ASN:ND2	1:A:23:LEU:HG	2.11	0.65
1:A:114:LYS:H	1:A:114:LYS:CD	2.07	0.65
1:A:251:MET:CE	1:A:255:SER:HB3	2.26	0.65
2:B:153:ILE:O	2:B:157:MET:HG3	1.96	0.65
2:B:157:MET:HE2	2:B:166:ILE:HD11	1.79	0.65
2:B:8:PHE:C	7:B:2001:HOH:O	2.33	0.65
2:B:38:GLU:OE1	2:B:38:GLU:HA	1.96	0.65
2:B:52:LYS:HE3	2:B:53:PHE:CE1	2.31	0.65
1:A:49:GLU:HA	1:A:52:LYS:CE	2.26	0.65
2:B:78:LYS:HA	2:B:81:TYR:HD2	1.62	0.64
2:B:141:THR:HG23	2:B:162:GLY:O	1.97	0.64
2:B:282:LYS:HE2	2:B:341:ILE:HG12	1.79	0.64
1:A:256:ARG:HG2	1:A:256:ARG:NH1	2.05	0.64
7:D:2005:HOH:O	4:F:10:DC:H2"	1.98	0.64
2:B:32:VAL:HG11	4:F:6:DG:H5'	1.80	0.64
1:A:208:ILE:CD1	1:A:212:LYS:HB3	2.28	0.64
2:B:23:LEU:O	2:B:26:LYS:HB2	1.97	0.64
1:A:96:SER:HB3	1:A:109:LEU:HD22	1.79	0.63
1:A:251:MET:HE1	1:A:255:SER:HB3	1.78	0.63
1:A:100:GLU:CB	1:A:108:TYR:HB2	2.22	0.63
1:A:118:TYR:O	1:A:121:ALA:N	2.31	0.63
2:B:256:ARG:NH1	2:B:328:ARG:O	2.32	0.63
4:F:8:DA:H2'	4:F:9:DT:C6	2.33	0.63
1:A:115:VAL:HG11	1:A:121:ALA:CA	2.29	0.63
1:A:261:ILE:CG2	1:A:319:LEU:HD21	2.29	0.63
2:B:125:GLY:O	2:B:129:LYS:HB2	1.99	0.63
2:B:136:GLU:HB3	2:B:138:ILE:HD13	1.81	0.63
4:E:5:O2G:H2'	4:E:6:DG:O5'	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:5:DG:H2"	3:C:6:DA:H8	1.62	0.63
2:B:256:ARG:HG2	2:B:256:ARG:NH2	2.12	0.63
2:B:289:VAL:HA	2:B:294:ASP:O	1.99	0.62
1:A:336:ARG:HH12	4:E:8:DA:H2'	1.63	0.62
1:A:197:LEU:HD13	1:A:212:LYS:HG3	1.81	0.62
1:A:210:PHE:HA	1:A:213:LEU:HD13	1.81	0.62
1:A:296:VAL:HG23	3:C:9:DG:OP1	2.00	0.62
3:C:4:DG:H2"	3:C:5:DG:C5'	2.22	0.62
1:A:17:GLU:OE2	1:A:24:LYS:HA	1.99	0.62
1:A:263:PRO:O	1:A:267:ARG:HG3	1.98	0.62
3:D:12:DT:H2"	3:D:13:DOC:O5'	2.00	0.62
1:A:167:ASP:N	1:A:167:ASP:OD1	2.32	0.62
1:A:99:ILE:HA	1:A:108:TYR:O	2.00	0.62
1:A:111:ILE:HG21	1:A:124:LEU:HD21	1.82	0.62
1:A:115:VAL:HG13	1:A:120:GLU:HB3	1.82	0.62
1:A:113:ASP:HB2	1:A:114:LYS:HD2	1.81	0.61
1:A:252:LYS:HD3	7:A:2006:HOH:O	2.00	0.61
4:E:3:DA:C2'	4:E:4:DC:C5'	2.78	0.61
1:A:257:ASN:HB3	1:A:260:GLU:HG3	1.82	0.61
1:A:280:ILE:CG2	1:A:341:ILE:HD12	2.31	0.61
2:B:119:ARG:O	2:B:119:ARG:HG2	2.01	0.61
1:A:208:ILE:CD1	1:A:212:LYS:CG	2.69	0.61
1:A:331:ARG:CZ	4:E:5:O2G:OP1	2.48	0.61
1:A:272:SER:O	1:A:276:LEU:HB2	2.01	0.60
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.83	0.60
1:A:318:LEU:O	1:A:322:ILE:HG13	2.01	0.60
2:B:37:PHE:CE2	2:B:40:SER:HB3	2.36	0.60
1:A:210:PHE:HA	1:A:213:LEU:CD1	2.32	0.60
1:A:291:GLU:O	1:A:293:LEU:HD22	2.02	0.60
2:B:189:ILE:O	2:B:193:LYS:HG3	2.01	0.60
2:B:84:VAL:O	2:B:88:ILE:HG13	2.01	0.60
1:A:244:SER:HB3	4:E:9:DT:OP2	2.02	0.60
4:E:3:DA:H2'	4:E:4:DC:C5'	2.32	0.60
1:A:142:VAL:HB	1:A:163:ILE:HG13	1.83	0.60
2:B:4:LEU:CD2	2:B:142:VAL:HG13	2.31	0.60
1:A:92:LEU:O	1:A:95:TYR:HB2	2.02	0.60
1:A:133:LEU:HA	1:A:138:ILE:O	2.02	0.60
2:B:57:ALA:CB	6:B:1345:TTP:H2'2	2.31	0.60
4:E:7:DA:H2"	4:E:8:DA:H5'	1.84	0.60
1:A:236:PRO:HG2	1:A:238:ARG:HH11	1.64	0.59
2:B:41:GLY:HA2	4:F:5:O2G:H5'	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:ARG:HG2	2:B:256:ARG:HH21	1.65	0.59
2:B:133:LEU:O	2:B:137:LYS:HD3	2.01	0.59
2:B:326:ASP:CG	2:B:327:GLU:N	2.55	0.59
2:B:147:ASN:HD22	2:B:233:TYR:HB3	1.67	0.59
2:B:146:LYS:HZ3	2:B:146:LYS:HB3	1.67	0.59
1:A:217:ILE:HD12	1:A:221:LYS:CG	2.32	0.59
2:B:256:ARG:NH1	2:B:328:ARG:C	2.57	0.59
2:B:319:LEU:HA	2:B:322:ILE:CD1	2.33	0.59
2:B:10:TYR:O	2:B:10:TYR:HD1	1.86	0.59
3:D:8:DG:H2"	3:D:9:DG:OP2	2.03	0.58
4:F:5:O2G:HM1B	4:F:6:DG:O4'	2.03	0.58
1:A:199:ILE:CG2	7:A:2035:HOH:O	2.33	0.58
4:F:7:DA:H2"	4:F:8:DA:O5'	2.02	0.58
1:A:329:LYS:NZ	7:A:2041:HOH:O	2.31	0.58
2:B:118:TYR:CE2	2:B:167:ASP:HA	2.39	0.58
1:A:98:LYS:NZ	1:A:110:ASP:CB	2.67	0.58
3:C:5:DG:H1	4:E:14:DC:H42	1.52	0.58
4:E:7:DA:H2"	4:E:8:DA:C5'	2.34	0.58
2:B:190:THR:HB	3:D:12:DT:OP1	2.03	0.58
1:A:136:GLU:O	1:A:137:LYS:HB2	2.03	0.58
3:C:2:DG:H1	4:E:17:DC:H42	1.52	0.58
1:A:293:LEU:HD22	1:A:293:LEU:N	2.19	0.58
2:B:247:ARG:HG2	2:B:271:GLU:HB2	1.85	0.57
1:A:262:LYS:NZ	1:A:316:VAL:HG11	2.19	0.57
2:B:4:LEU:HD21	2:B:142:VAL:CG1	2.34	0.57
1:A:293:LEU:HD11	1:A:331:ARG:HH11	1.69	0.57
1:A:123:ASN:C	1:A:125:GLY:N	2.58	0.57
2:B:195:LYS:CA	7:B:2027:HOH:O	2.36	0.57
1:A:166:ILE:HG12	1:A:170:GLU:OE2	2.04	0.57
1:A:166:ILE:HG23	1:A:170:GLU:HB3	1.86	0.57
2:B:258:LEU:O	2:B:259:GLU:C	2.43	0.57
1:A:290:THR:OG1	1:A:294:ASP:HB3	2.05	0.57
2:B:259:GLU:O	2:B:262:LYS:HG2	2.05	0.57
1:A:51:ARG:C	1:A:53:PHE:H	2.08	0.57
1:A:209:GLU:HB2	1:A:212:LYS:HB2	1.87	0.57
1:A:47:ASN:CG	1:A:49:GLU:HG2	2.24	0.57
1:A:204:ASP:CA	7:A:2035:HOH:O	2.52	0.57
2:B:117:ASP:OD2	2:B:120:GLU:HB2	2.05	0.57
2:B:244:SER:O	2:B:245:ILE:HD13	2.04	0.57
2:B:258:LEU:CD1	2:B:259:GLU:CA	2.81	0.57
2:B:10:TYR:CB	2:B:51:ARG:NH1	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:TYR:HB2	2:B:51:ARG:NH1	2.20	0.56
2:B:88:ILE:HG23	2:B:132:ILE:HG23	1.86	0.56
3:C:4:DG:N7	7:C:2004:HOH:O	2.33	0.56
1:A:280:ILE:HG21	1:A:341:ILE:HD12	1.87	0.56
2:B:19:LEU:CD2	2:B:77:ARG:HH22	2.18	0.56
1:A:10:TYR:HA	6:A:1345:TTP:O2G	2.05	0.56
2:B:319:LEU:O	2:B:323:LEU:HG	2.05	0.56
4:E:5:O2G:H2'	4:E:6:DG:C5'	2.36	0.56
1:A:47:ASN:OD1	1:A:49:GLU:HG2	2.04	0.56
1:A:124:LEU:O	1:A:128:ILE:HD12	2.05	0.56
2:B:37:PHE:HD1	2:B:38:GLU:N	2.04	0.56
1:A:72:VAL:HG12	1:A:74:LEU:HG	1.88	0.56
1:A:8:PHE:CE1	1:A:88:ILE:HG21	2.41	0.56
1:A:197:LEU:HD21	1:A:216:MET:SD	2.46	0.56
2:B:123:ASN:HA	2:B:126:LEU:HD12	1.87	0.56
1:A:115:VAL:HG11	1:A:121:ALA:HA	1.88	0.56
2:B:148:LYS:HD3	2:B:237:ILE:CG1	2.28	0.56
1:A:250:THR:CG2	1:A:332:ARG:HD2	2.36	0.55
1:A:336:ARG:NH2	4:E:8:DA:OP2	2.40	0.55
1:A:123:ASN:C	1:A:125:GLY:H	2.10	0.55
1:A:259:GLU:OE1	1:A:259:GLU:HA	2.06	0.55
2:B:136:GLU:HB3	2:B:138:ILE:CD1	2.37	0.55
2:B:199:ILE:HD11	2:B:208:ILE:HG13	1.88	0.55
1:A:144:ILE:CG2	1:A:165:VAL:HG23	2.35	0.55
1:A:153:ILE:HG22	1:A:157:MET:CE	2.36	0.55
2:B:1:MET:N	7:B:2016:HOH:O	2.29	0.55
2:B:12:TYR:HB2	2:B:45:THR:HG23	1.87	0.55
2:B:256:ARG:HB2	2:B:329:LYS:HA	1.88	0.55
1:A:237:ILE:C	1:A:238:ARG:HG2	2.27	0.55
2:B:11:PHE:O	2:B:15:VAL:HG23	2.07	0.55
2:B:228:LEU:HD23	2:B:233:TYR:HB2	1.89	0.55
2:B:283:ALA:HB2	2:B:339:LYS:HD2	1.88	0.55
2:B:326:ASP:O	2:B:327:GLU:HG2	2.06	0.55
1:A:9:ASP:O	1:A:10:TYR:C	2.45	0.55
1:A:133:LEU:CD2	7:A:2026:HOH:O	2.25	0.55
1:A:193:LYS:HB3	1:A:216:MET:HG2	1.88	0.55
1:A:202:LEU:O	1:A:205:THR:HG23	2.06	0.55
2:B:241:VAL:O	2:B:243:LYS:HE3	2.06	0.55
1:A:280:ILE:HG23	1:A:305:GLY:HA3	1.87	0.55
1:A:332:ARG:HG3	1:A:332:ARG:HH11	1.70	0.55
2:B:254:ASN:O	2:B:255:SER:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:LEU:HD11	2:B:182:ASP:HB2	1.87	0.55
1:A:251:MET:CE	1:A:261:ILE:HG12	2.34	0.55
3:C:8:DG:H2"	3:C:9:DG:OP2	2.07	0.55
1:A:336:ARG:HH22	4:E:8:DA:H5'	1.72	0.54
2:B:2:ILE:HG22	2:B:111:ILE:HG12	1.89	0.54
1:A:200:ASN:CB	1:A:201:LYS:HZ3	2.17	0.54
1:A:268:ALA:HB1	1:A:335:VAL:HG22	1.88	0.54
2:B:243:LYS:N	4:F:9:DT:OP1	2.37	0.54
2:B:115:VAL:HG11	2:B:121:ALA:HA	1.89	0.54
2:B:166:ILE:HG23	2:B:170:GLU:HB3	1.88	0.54
2:B:289:VAL:HG21	2:B:332:ARG:HG3	1.89	0.54
1:A:23:LEU:HD22	1:A:72:VAL:HG21	1.89	0.54
1:A:27:PRO:HA	1:A:49:GLU:HB2	1.89	0.54
1:A:293:LEU:HD22	1:A:293:LEU:H	1.71	0.54
2:B:147:ASN:ND2	2:B:233:TYR:HB3	2.23	0.54
1:A:29:VAL:HG21	1:A:73:TYR:CD2	2.43	0.54
2:B:82:GLN:O	2:B:82:GLN:NE2	2.41	0.54
2:B:266:PHE:HB3	2:B:312:TYR:CE1	2.43	0.54
1:A:245:ILE:HG22	1:A:246:GLY:N	2.22	0.54
1:A:296:VAL:O	1:A:296:VAL:HG13	2.08	0.54
2:B:1:MET:HA	2:B:112:SER:OG	2.06	0.54
2:B:241:VAL:HG12	2:B:242:ARG:N	2.22	0.54
2:B:251:MET:HG2	2:B:264:TYR:CD2	2.43	0.54
2:B:256:ARG:O	2:B:256:ARG:CD	2.55	0.54
1:A:85:SER:O	1:A:89:MET:HG2	2.07	0.54
1:A:189:ILE:HB	3:C:11:DT:H3'	1.90	0.54
2:B:233:TYR:O	2:B:234:ASN:O	2.25	0.54
2:B:314:GLU:OE2	2:B:317:LYS:HD2	2.07	0.54
2:B:61:ILE:O	2:B:65:LYS:HG3	2.08	0.53
1:A:199:ILE:HG23	1:A:204:ASP:HB2	1.89	0.53
1:A:189:ILE:HD13	7:A:2033:HOH:O	2.08	0.53
2:B:37:PHE:CD1	2:B:38:GLU:N	2.77	0.53
6:B:1345:TTP:O1B	6:B:1345:TTP:O1A	2.26	0.53
1:A:57:ALA:HB3	6:A:1345:TTP:H2'2	1.90	0.53
2:B:256:ARG:O	2:B:256:ARG:CG	2.56	0.53
1:A:114:LYS:HD2	1:A:114:LYS:N	2.16	0.53
1:A:159:LYS:NZ	6:A:1345:TTP:O1B	2.37	0.53
1:A:222:ALA:C	1:A:226:ILE:HD12	2.28	0.53
2:B:250:THR:HG23	2:B:332:ARG:HD2	1.91	0.53
2:B:257:ASN:O	2:B:258:LEU:C	2.47	0.53
1:A:91:LEU:HD11	1:A:135:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HA	1:A:112:SER:OG	2.08	0.53
2:B:122:TYR:CE2	2:B:126:LEU:HD11	2.43	0.53
1:A:158:ALA:O	1:A:162:GLY:HA3	2.09	0.53
1:A:269:ILE:HG21	1:A:312:TYR:CE2	2.43	0.52
2:B:109:LEU:O	2:B:111:ILE:CD1	2.57	0.52
2:B:254:ASN:OD1	2:B:331:ARG:HA	2.09	0.52
2:B:300:ARG:HH11	2:B:314:GLU:CD	2.13	0.52
2:B:338:SER:HA	2:B:340:PHE:CE1	2.44	0.52
2:B:209:GLU:HB2	2:B:212:LYS:HE3	1.90	0.52
2:B:114:LYS:O	2:B:115:VAL:CB	2.57	0.52
1:A:26:LYS:O	1:A:49:GLU:HG3	2.10	0.52
1:A:93:ARG:C	1:A:95:TYR:H	2.12	0.52
1:A:175:ILE:O	1:A:203:VAL:HG12	2.10	0.52
1:A:262:LYS:HZ1	1:A:316:VAL:HG11	1.73	0.52
2:B:135:LYS:O	2:B:136:GLU:HG2	2.10	0.52
2:B:10:TYR:CE1	2:B:14:GLN:HB2	2.44	0.52
2:B:89:MET:O	2:B:91:LEU:N	2.42	0.52
2:B:293:LEU:HD11	4:F:4:DC:H2'	1.92	0.52
2:B:147:ASN:CB	2:B:233:TYR:CD2	2.92	0.52
1:A:270:GLU:OE1	1:A:312:TYR:OH	2.28	0.52
1:A:312:TYR:O	1:A:316:VAL:HG23	2.10	0.52
2:B:226:ILE:O	2:B:229:ALA:HB3	2.09	0.52
4:F:17:DC:H1'	7:F:2006:HOH:O	2.10	0.52
1:A:9:ASP:O	1:A:11:PHE:N	2.43	0.52
1:A:157:MET:CE	1:A:166:ILE:HD11	2.40	0.52
1:A:115:VAL:HG11	1:A:121:ALA:N	2.25	0.52
2:B:115:VAL:HG12	2:B:115:VAL:O	2.09	0.52
2:B:296:VAL:HG23	3:D:9:DG:OP1	2.09	0.52
1:A:293:LEU:HD11	1:A:331:ARG:NH1	2.26	0.51
3:D:10:DA:H1'	7:D:2006:HOH:O	2.10	0.51
1:A:100:GLU:O	1:A:108:TYR:N	2.44	0.51
1:A:204:ASP:CB	7:A:2035:HOH:O	2.38	0.51
1:A:287:VAL:O	1:A:333:ILE:HD12	2.09	0.51
2:B:196:LYS:C	2:B:198:GLY:H	2.14	0.51
2:B:254:ASN:O	2:B:255:SER:CB	2.57	0.51
2:B:290:THR:CG2	2:B:328:ARG:HB3	2.40	0.51
1:A:49:GLU:O	1:A:52:LYS:HG2	2.09	0.51
1:A:111:ILE:HG21	1:A:124:LEU:CD2	2.41	0.51
1:A:157:MET:SD	1:A:164:LYS:HE3	2.50	0.51
1:A:227:SER:OG	1:A:233:TYR:HA	2.11	0.51
2:B:320:GLN:C	2:B:322:ILE:H	2.14	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HA	1:A:52:LYS:CD	2.40	0.51
1:A:98:LYS:NZ	1:A:110:ASP:OD1	2.43	0.51
1:A:281:PRO:O	1:A:306:ILE:HG13	2.11	0.51
1:A:49:GLU:HA	1:A:52:LYS:HD3	1.93	0.51
2:B:68:LEU:C	2:B:70:ASN:H	2.14	0.51
1:A:250:THR:HG22	1:A:332:ARG:HD2	1.93	0.51
2:B:115:VAL:HG11	2:B:120:GLU:C	2.32	0.51
2:B:262:LYS:HB2	2:B:263:PRO:CD	2.41	0.51
2:B:326:ASP:C	2:B:327:GLU:HG2	2.31	0.51
7:B:2033:HOH:O	3:D:7:DA:C8	2.54	0.51
1:A:148:LYS:O	1:A:151:ALA:HB3	2.11	0.51
1:A:294:ASP:OD2	1:A:328:ARG:NH2	2.42	0.51
2:B:1:MET:HE2	2:B:146:LYS:O	2.10	0.51
2:B:141:THR:HA	2:B:162:GLY:O	2.11	0.51
2:B:208:ILE:HG22	2:B:209:GLU:N	2.26	0.51
1:A:209:GLU:O	1:A:213:LEU:HD12	2.11	0.50
2:B:11:PHE:HE2	2:B:104:ILE:HG12	1.74	0.50
2:B:105:ASP:C	2:B:106:GLU:HG3	2.32	0.50
2:B:106:GLU:OE2	2:B:152:LYS:NZ	2.44	0.50
2:B:176:ARG:HA	2:B:203:VAL:CG1	2.42	0.50
4:F:14:DC:H2"	4:F:15:DC:O4'	2.11	0.50
1:A:111:ILE:HD12	1:A:115:VAL:HB	1.93	0.50
2:B:89:MET:C	2:B:91:LEU:H	2.13	0.50
1:A:126:LEU:HA	1:A:129:LYS:HB3	1.92	0.50
1:A:276:LEU:HD22	1:A:279:ARG:HB2	1.93	0.50
1:A:291:GLU:OE1	1:A:291:GLU:HA	2.11	0.50
1:A:181:ALA:HA	1:A:186:ILE:HG21	1.94	0.50
1:A:258:LEU:O	1:A:262:LYS:HG3	2.12	0.50
2:B:3:VAL:HG11	2:B:148:LYS:HA	1.93	0.50
2:B:100:GLU:HG3	2:B:238:ARG:O	2.11	0.50
2:B:144:ILE:O	2:B:145:SER:HB2	2.12	0.50
1:A:180:ILE:N	1:A:200:ASN:O	2.45	0.50
1:A:210:PHE:CD1	1:A:226:ILE:HD11	2.46	0.50
1:A:191:ALA:O	1:A:195:LYS:HD3	2.12	0.50
2:B:5:PHE:CE2	2:B:152:LYS:HD2	2.46	0.50
2:B:92:LEU:HB3	2:B:109:LEU:HD11	1.93	0.50
1:A:48:TYR:N	1:A:48:TYR:CD2	2.76	0.50
1:A:202:LEU:O	1:A:204:ASP:N	2.45	0.50
2:B:122:TYR:CG	2:B:122:TYR:O	2.65	0.50
2:B:233:TYR:CD2	2:B:234:ASN:N	2.80	0.50
2:B:257:ASN:HB3	2:B:260:GLU:CD	2.32	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:CYS:HB2	1:A:42:ALA:O	2.12	0.49
1:A:92:LEU:CD2	1:A:132:ILE:HD11	2.42	0.49
1:A:218:GLY:HA2	4:E:12:DT:OP1	2.12	0.49
2:B:4:LEU:CB	2:B:111:ILE:CD1	2.83	0.49
2:B:68:LEU:O	2:B:70:ASN:N	2.45	0.49
1:A:51:ARG:O	1:A:53:PHE:N	2.45	0.49
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.77	0.49
2:B:46:ALA:HB1	2:B:50:ALA:HB3	1.94	0.49
2:B:186:ILE:HD11	2:B:225:LEU:HD21	1.92	0.49
2:B:317:LYS:HB2	2:B:317:LYS:NZ	2.27	0.49
2:B:258:LEU:HD13	2:B:259:GLU:CA	2.39	0.49
2:B:247:ARG:O	2:B:268:ALA:HB1	2.13	0.49
2:B:258:LEU:HD12	2:B:259:GLU:CA	2.42	0.49
2:B:286:VAL:HG22	2:B:335:VAL:HG12	1.94	0.49
2:B:323:LEU:HD21	2:B:330:ILE:HD12	1.94	0.49
1:A:93:ARG:HH12	1:A:101:ILE:HD11	1.76	0.49
1:A:108:TYR:CE2	1:A:148:LYS:HB3	2.47	0.49
2:B:48:TYR:CE1	2:B:160:PRO:HD3	2.48	0.49
1:A:170:GLU:C	1:A:172:LYS:N	2.64	0.49
1:A:256:ARG:CG	1:A:256:ARG:NH1	2.66	0.49
1:A:269:ILE:HG21	1:A:312:TYR:HE2	1.77	0.49
1:A:327:GLU:N	1:A:327:GLU:CD	2.66	0.49
1:A:170:GLU:HG3	1:A:173:ARG:HH22	1.76	0.49
1:A:166:ILE:HG22	1:A:166:ILE:O	2.13	0.48
1:A:218:GLY:CA	4:E:12:DT:OP1	2.61	0.48
2:B:32:VAL:HG11	4:F:6:DG:C5'	2.42	0.48
2:B:269:ILE:HA	2:B:335:VAL:HG21	1.94	0.48
1:A:1:MET:H2	1:A:116:ARG:HH12	1.61	0.48
1:A:193:LYS:HB3	1:A:216:MET:HG3	1.91	0.48
2:B:251:MET:HG2	2:B:264:TYR:CG	2.49	0.48
2:B:319:LEU:O	2:B:322:ILE:HB	2.13	0.48
1:A:328:ARG:HG2	1:A:328:ARG:NH1	2.29	0.48
2:B:9:ASP:CG	2:B:161:ASN:H	2.16	0.48
2:B:202:LEU:HD23	2:B:202:LEU:O	2.13	0.48
2:B:237:ILE:HG22	2:B:237:ILE:O	2.13	0.48
3:C:7:DA:H2"	3:C:8:DG:C8	2.48	0.48
1:A:7:ASP:HA	1:A:105:ASP:O	2.13	0.48
1:A:32:VAL:CG1	1:A:76:MET:CE	2.90	0.48
2:B:14:GLN:O	2:B:15:VAL:C	2.49	0.48
1:A:243:LYS:O	1:A:244:SER:HB2	2.14	0.48
3:D:11:DT:H2"	3:D:12:DT:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ALA:O	1:A:51:ARG:NE	2.47	0.48
2:B:9:ASP:O	2:B:10:TYR:C	2.51	0.48
2:B:321:LYS:O	2:B:325:GLU:HB3	2.14	0.48
4:F:5:O2G:H2'	4:F:6:DG:O5'	2.14	0.48
1:A:10:TYR:CE1	1:A:14:GLN:HB2	2.48	0.48
1:A:49:GLU:OE2	1:A:49:GLU:N	2.46	0.48
1:A:173:ARG:O	1:A:177:GLU:CG	2.61	0.48
1:A:291:GLU:C	1:A:293:LEU:H	2.18	0.48
1:A:195:LYS:HE2	1:A:200:ASN:OD1	2.14	0.47
2:B:2:ILE:CG2	2:B:111:ILE:HG12	2.44	0.47
2:B:289:VAL:HB	2:B:332:ARG:CG	2.44	0.47
2:B:38:GLU:O	2:B:39:ASP:CB	2.62	0.47
3:C:5:DG:H1	4:E:14:DC:N4	2.13	0.47
4:E:8:DA:H2"	4:E:9:DT:C6	2.49	0.47
1:A:153:ILE:HD13	1:A:178:LEU:CD2	2.45	0.47
1:A:265:LEU:HD22	1:A:319:LEU:HD22	1.96	0.47
4:F:16:DC:H2"	4:F:17:DC:O4'	2.15	0.47
1:A:48:TYR:O	1:A:52:LYS:HD3	2.14	0.47
1:A:62:VAL:O	1:A:66:LYS:HD3	2.15	0.47
1:A:98:LYS:CE	1:A:110:ASP:HB3	2.44	0.47
1:A:257:ASN:O	1:A:259:GLU:N	2.47	0.47
2:B:110:ASP:HB2	2:B:237:ILE:CD1	2.34	0.47
2:B:281:PRO:O	2:B:306:ILE:HG13	2.14	0.47
1:A:280:ILE:CG2	1:A:341:ILE:CD1	2.92	0.47
2:B:78:LYS:NZ	7:B:2011:HOH:O	2.46	0.47
3:D:6:DA:H2"	3:D:7:DA:OP2	2.13	0.47
1:A:176:ARG:HA	1:A:203:VAL:HG12	1.96	0.47
1:A:280:ILE:HG22	1:A:341:ILE:CD1	2.45	0.47
2:B:63:GLU:O	2:B:66:LYS:N	2.47	0.47
2:B:89:MET:C	2:B:91:LEU:N	2.68	0.47
1:A:4:LEU:C	1:A:4:LEU:HD23	2.35	0.47
1:A:19:LEU:O	1:A:20:ASN:CB	2.62	0.47
1:A:29:VAL:CG1	1:A:55:VAL:HG11	2.44	0.47
1:A:61:ILE:O	1:A:64:ALA:HB3	2.13	0.47
1:A:327:GLU:N	1:A:327:GLU:OE2	2.48	0.47
2:B:21:PRO:C	2:B:23:LEU:H	2.17	0.47
2:B:257:ASN:O	2:B:258:LEU:O	2.33	0.47
3:C:8:DG:H2"	3:C:9:DG:C8	2.50	0.47
1:A:166:ILE:HG23	1:A:170:GLU:CG	2.45	0.47
1:A:276:LEU:O	1:A:277:ASP:C	2.53	0.47
2:B:93:ARG:HG3	2:B:93:ARG:HH11	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:VAL:HG21	4:E:5:O2G:H1'	1.96	0.47
1:A:119:ARG:O	1:A:123:ASN:ND2	2.48	0.47
1:A:238:ARG:NH1	1:A:238:ARG:HG3	2.29	0.47
1:A:46:ALA:HB1	1:A:50:ALA:HB3	1.96	0.47
1:A:60:PRO:HG2	4:E:3:DA:N3	2.30	0.47
2:B:157:MET:CE	2:B:166:ILE:HD11	2.44	0.47
2:B:261:ILE:N	2:B:261:ILE:HD12	2.30	0.47
2:B:255:SER:O	2:B:330:ILE:N	2.46	0.46
1:A:1:MET:H1	1:A:116:ARG:HH12	1.63	0.46
2:B:88:ILE:CG2	2:B:132:ILE:HD13	2.45	0.46
2:B:241:VAL:CG1	2:B:242:ARG:N	2.77	0.46
1:A:48:TYR:O	1:A:52:LYS:HB3	2.16	0.46
2:B:138:ILE:N	2:B:138:ILE:HD12	2.30	0.46
2:B:203:VAL:HG13	2:B:204:ASP:N	2.30	0.46
2:B:298:ARG:HG2	2:B:298:ARG:HH11	1.79	0.46
1:A:95:TYR:O	1:A:96:SER:HB2	2.14	0.46
1:A:254:ASN:CG	1:A:291:GLU:HG2	2.36	0.46
1:A:270:GLU:C	1:A:272:SER:H	2.19	0.46
2:B:142:VAL:O	2:B:163:ILE:HA	2.15	0.46
1:A:76:MET:HG3	1:A:81:TYR:HE2	1.80	0.46
1:A:100:GLU:HB2	1:A:237:ILE:HG23	1.97	0.46
2:B:92:LEU:C	2:B:94:GLU:H	2.19	0.46
2:B:259:GLU:HA	2:B:262:LYS:CG	2.46	0.46
1:A:173:ARG:HB3	1:A:173:ARG:NH1	2.29	0.46
1:A:176:ARG:HA	1:A:203:VAL:CG1	2.46	0.46
2:B:111:ILE:H	2:B:111:ILE:CD1	2.08	0.46
2:B:164:LYS:HG3	2:B:165:VAL:H	1.80	0.46
2:B:210:PHE:O	2:B:214:LYS:HB3	2.15	0.46
2:B:256:ARG:NH1	2:B:328:ARG:CA	2.78	0.46
2:B:271:GLU:O	2:B:275:LYS:HG3	2.16	0.46
2:B:82:GLN:NE2	2:B:82:GLN:CA	2.78	0.46
2:B:166:ILE:O	2:B:166:ILE:HG22	2.15	0.46
2:B:217:ILE:HD12	2:B:221:LYS:HB3	1.96	0.46
2:B:258:LEU:HD11	2:B:262:LYS:HE3	0.63	0.46
2:B:302:PHE:HZ	2:B:314:GLU:HG2	1.80	0.46
1:A:180:ILE:HG22	1:A:195:LYS:CE	2.46	0.46
1:A:8:PHE:CZ	1:A:88:ILE:HG21	2.50	0.46
1:A:63:GLU:O	1:A:66:LYS:HB2	2.15	0.46
1:A:257:ASN:HB3	1:A:260:GLU:CG	2.45	0.46
2:B:139:THR:HG21	2:B:161:ASN:ND2	2.31	0.46
1:A:79:GLU:O	1:A:82:GLN:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ARG:HD2	1:A:340:PHE:CE2	2.51	0.45
2:B:202:LEU:O	2:B:229:ALA:CB	2.64	0.45
2:B:276:LEU:HD22	2:B:279:ARG:O	2.15	0.45
2:B:209:GLU:HA	2:B:209:GLU:OE1	2.16	0.45
2:B:287:VAL:O	2:B:333:ILE:HD12	2.16	0.45
4:F:16:DC:C2'	4:F:17:DC:C6	2.95	0.45
1:A:84:VAL:O	1:A:84:VAL:HG12	2.17	0.45
1:A:173:ARG:HH11	1:A:173:ARG:CB	2.30	0.45
2:B:9:ASP:HB2	2:B:139:THR:O	2.16	0.45
2:B:37:PHE:CZ	2:B:40:SER:HA	2.52	0.45
1:A:245:ILE:CG2	1:A:246:GLY:N	2.79	0.45
1:A:247:ARG:HG3	1:A:247:ARG:HH11	1.82	0.45
2:B:154:ALA:HB1	2:B:164:LYS:HB3	1.98	0.45
1:A:29:VAL:HG11	1:A:55:VAL:HG11	1.98	0.45
1:A:255:SER:OG	1:A:260:GLU:HB2	2.16	0.45
2:B:290:THR:HG21	2:B:328:ARG:NE	2.32	0.45
1:A:98:LYS:HB2	1:A:98:LYS:HE3	1.52	0.45
1:A:180:ILE:CG2	1:A:195:LYS:HE3	2.45	0.45
2:B:48:TYR:CE2	2:B:160:PRO:HB3	2.52	0.45
1:A:7:ASP:OD2	6:A:1345:TTP:O1B	2.34	0.45
1:A:285:HIS:HA	1:A:299:GLY:HA2	1.99	0.45
1:A:121:ALA:HB1	1:A:144:ILE:HD13	1.99	0.45
2:B:164:LYS:CG	2:B:165:VAL:N	2.79	0.45
2:B:183:VAL:HG22	2:B:202:LEU:HD12	1.98	0.45
1:A:48:TYR:CE1	1:A:160:PRO:HD3	2.52	0.45
1:A:217:ILE:HD12	1:A:221:LYS:HB3	1.99	0.45
1:A:252:LYS:HA	1:A:252:LYS:CE	2.44	0.45
1:A:322:ILE:C	1:A:324:GLU:N	2.71	0.45
2:B:289:VAL:HB	2:B:332:ARG:HG2	1.99	0.45
3:C:9:DG:OP2	3:C:9:DG:H8	1.99	0.45
1:A:37:PHE:CD2	1:A:37:PHE:N	2.85	0.44
2:B:115:VAL:HG11	2:B:121:ALA:CA	2.46	0.44
1:A:23:LEU:O	1:A:25:GLY:N	2.50	0.44
1:A:331:ARG:NH2	4:E:4:DC:H3'	2.29	0.44
2:B:2:ILE:HD12	2:B:2:ILE:N	2.32	0.44
2:B:248:ILE:CD1	7:B:2035:HOH:O	2.64	0.44
1:A:166:ILE:HG23	1:A:170:GLU:CD	2.38	0.44
1:A:279:ARG:HD2	1:A:340:PHE:CD2	2.53	0.44
2:B:256:ARG:HH12	2:B:328:ARG:CA	2.24	0.44
1:A:71:ALA:HB3	1:A:73:TYR:CE1	2.52	0.44
2:B:156:ASP:HA	2:B:159:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:7:DA:C2'	4:F:8:DA:O5'	2.66	0.44
1:A:19:LEU:O	1:A:20:ASN:HB2	2.17	0.44
1:A:157:MET:HE1	1:A:166:ILE:HD11	2.00	0.44
1:A:232:GLU:O	1:A:234:ASN:N	2.51	0.44
1:A:247:ARG:HD3	1:A:271:GLU:CG	2.36	0.44
1:A:256:ARG:HB2	1:A:329:LYS:HZ2	1.83	0.44
1:A:20:ASN:OD1	7:A:2002:HOH:O	2.21	0.44
1:A:244:SER:O	1:A:245:ILE:HD13	2.17	0.44
2:B:89:MET:O	2:B:92:LEU:N	2.39	0.44
2:B:175:ILE:HG22	2:B:203:VAL:HB	1.99	0.44
1:A:249:VAL:HG21	1:A:264:TYR:HB3	2.00	0.44
2:B:93:ARG:HB2	2:B:93:ARG:CZ	2.48	0.44
2:B:232:GLU:O	2:B:232:GLU:HG2	2.17	0.44
3:D:3:DG:H2"	3:D:4:DG:O5'	2.18	0.44
1:A:322:ILE:C	1:A:324:GLU:H	2.20	0.44
4:F:12:DT:H2"	4:F:13:DT:O4'	2.18	0.44
1:A:99:ILE:HG13	1:A:108:TYR:O	2.18	0.44
1:A:221:LYS:O	1:A:224:TYR:HB3	2.18	0.44
1:A:230:ARG:C	1:A:232:GLU:H	2.21	0.44
1:A:236:PRO:O	1:A:238:ARG:HG2	2.17	0.44
1:A:49:GLU:HA	1:A:52:LYS:HE2	1.97	0.43
1:A:62:VAL:HG23	1:A:63:GLU:N	2.33	0.43
2:B:65:LYS:O	2:B:69:PRO:HD3	2.18	0.43
1:A:256:ARG:HB2	1:A:329:LYS:HG3	1.99	0.43
2:B:266:PHE:CD1	2:B:312:TYR:CD1	3.06	0.43
1:A:49:GLU:O	1:A:52:LYS:HE2	2.17	0.43
1:A:288:ALA:HB2	1:A:333:ILE:CD1	2.48	0.43
2:B:296:VAL:CG2	2:B:298:ARG:HH12	2.31	0.43
1:A:29:VAL:HG23	1:A:29:VAL:O	2.18	0.43
1:A:171:VAL:O	1:A:171:VAL:CG1	2.64	0.43
1:A:234:ASN:OD1	1:A:234:ASN:C	2.57	0.43
2:B:6:VAL:HG13	2:B:140:VAL:HG21	2.00	0.43
2:B:173:ARG:HH11	2:B:173:ARG:HG3	1.83	0.43
2:B:194:LEU:O	2:B:199:ILE:O	2.36	0.43
2:B:222:ALA:C	2:B:224:TYR:N	2.71	0.43
2:B:282:LYS:HE2	2:B:341:ILE:CG1	2.47	0.43
2:B:298:ARG:HA	3:D:8:DG:OP2	2.18	0.43
2:B:322:ILE:O	2:B:326:ASP:N	2.51	0.43
1:A:99:ILE:CA	1:A:108:TYR:O	2.64	0.43
2:B:88:ILE:HG23	2:B:132:ILE:CG2	2.48	0.43
2:B:111:ILE:O	2:B:113:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ILE:CG2	2:B:193:LYS:HE3	2.48	0.43
2:B:290:THR:OG1	2:B:294:ASP:HB3	2.18	0.43
2:B:115:VAL:HG11	2:B:121:ALA:N	2.34	0.43
2:B:189:ILE:HB	3:D:12:DT:OP2	2.18	0.43
2:B:311:ALA:C	2:B:313:SER:H	2.22	0.43
4:E:5:O2G:H2'	4:E:6:DG:H5'	2.00	0.43
1:A:333:ILE:HG23	1:A:333:ILE:O	2.19	0.43
2:B:205:THR:C	2:B:207:SER:N	2.72	0.43
4:F:12:DT:H2'	4:F:13:DT:C6	2.53	0.43
1:A:280:ILE:CG2	1:A:305:GLY:CA	2.93	0.43
1:A:308:LYS:O	1:A:311:ALA:HB3	2.19	0.43
2:B:205:THR:C	2:B:207:SER:H	2.22	0.43
2:B:258:LEU:CD1	2:B:259:GLU:HA	2.49	0.43
1:A:110:ASP:C	1:A:112:SER:H	2.22	0.43
1:A:193:LYS:HD3	1:A:216:MET:O	2.19	0.43
2:B:59:ILE:HD12	2:B:63:GLU:CB	2.46	0.43
1:A:84:VAL:O	1:A:88:ILE:HG13	2.19	0.42
1:A:151:ALA:O	1:A:154:ALA:HB3	2.19	0.42
1:A:51:ARG:NH2	6:A:1345:TTP:O2G	2.51	0.42
1:A:199:ILE:HG22	1:A:200:ASN:N	2.34	0.42
2:B:149:VAL:O	2:B:153:ILE:HG13	2.19	0.42
3:D:4:DG:C2	3:D:5:DG:C5	3.07	0.42
1:A:237:ILE:N	1:A:237:ILE:HD12	2.34	0.42
2:B:10:TYR:HD1	2:B:13:ALA:HB3	1.84	0.42
2:B:130:ASN:O	2:B:134:GLU:HB2	2.18	0.42
2:B:159:LYS:HE2	6:B:1345:TTP:O2B	2.19	0.42
2:B:192:GLU:CD	7:B:2026:HOH:O	2.56	0.42
2:B:249:VAL:O	2:B:332:ARG:HA	2.19	0.42
2:B:320:GLN:C	2:B:322:ILE:N	2.73	0.42
3:D:9:DG:H2"	3:D:10:DA:O5'	2.19	0.42
1:A:213:LEU:O	1:A:216:MET:N	2.46	0.42
2:B:161:ASN:OD1	2:B:161:ASN:O	2.37	0.42
2:B:180:ILE:HA	2:B:183:VAL:HG23	2.02	0.42
2:B:202:LEU:O	2:B:229:ALA:HB2	2.18	0.42
1:A:192:GLU:O	1:A:195:LYS:N	2.52	0.42
2:B:197:LEU:HD13	2:B:213:LEU:HD23	2.02	0.42
2:B:197:LEU:CD1	2:B:213:LEU:HD23	2.49	0.42
4:F:3:DA:H2"	4:F:4:DC:H5'	2.02	0.42
1:A:47:ASN:ND2	1:A:49:GLU:HG2	2.34	0.42
1:A:194:LEU:HD21	1:A:217:ILE:HG21	2.02	0.42
1:A:289:VAL:HB	1:A:332:ARG:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:269:ILE:O	2:B:273:TYR:HB2	2.19	0.42
4:F:9:DT:H2'	4:F:10:DC:C6	2.54	0.42
1:A:99:ILE:CG1	1:A:108:TYR:O	2.68	0.42
1:A:175:ILE:HG22	1:A:203:VAL:HB	2.02	0.42
1:A:23:LEU:CD2	1:A:72:VAL:HG21	2.49	0.42
1:A:126:LEU:O	1:A:130:ASN:CB	2.66	0.42
1:A:169:GLU:O	1:A:169:GLU:HG2	2.19	0.42
1:A:192:GLU:O	1:A:193:LYS:C	2.58	0.42
1:A:256:ARG:HH21	1:A:327:GLU:CA	2.15	0.42
2:B:72:VAL:HG12	2:B:74:LEU:HD21	2.02	0.42
2:B:251:MET:HA	2:B:264:TYR:CE1	2.55	0.42
3:C:2:DG:H2"	3:C:3:DG:C8	2.55	0.42
1:A:6:VAL:CG1	1:A:140:VAL:HG21	2.50	0.42
1:A:76:MET:HE3	1:A:76:MET:HB3	1.92	0.42
1:A:204:ASP:C	7:A:2035:HOH:O	2.58	0.42
2:B:276:LEU:O	2:B:279:ARG:CZ	2.67	0.42
2:B:32:VAL:CG2	4:F:5:O2G:HM1A	2.46	0.42
2:B:63:GLU:O	2:B:64:ALA:C	2.57	0.42
2:B:82:GLN:HE21	2:B:82:GLN:C	2.24	0.42
1:A:98:LYS:HZ1	1:A:110:ASP:CB	2.33	0.41
1:A:166:ILE:O	1:A:167:ASP:C	2.58	0.41
2:B:199:ILE:CD1	2:B:208:ILE:HG13	2.50	0.41
2:B:324:GLU:O	2:B:324:GLU:HG2	2.15	0.41
1:A:205:THR:N	7:A:2035:HOH:O	2.54	0.41
2:B:71:ALA:HB3	2:B:73:TYR:CE1	2.55	0.41
2:B:86:SER:O	2:B:90:ASN:ND2	2.53	0.41
2:B:159:LYS:HB3	2:B:159:LYS:HE3	1.82	0.41
2:B:175:ILE:HG21	2:B:229:ALA:O	2.20	0.41
2:B:136:GLU:O	2:B:137:LYS:HB2	2.20	0.41
2:B:266:PHE:HB3	2:B:312:TYR:HE1	1.85	0.41
2:B:63:GLU:OE1	2:B:63:GLU:HA	2.20	0.41
2:B:136:GLU:O	2:B:138:ILE:HD12	2.20	0.41
1:A:51:ARG:C	1:A:53:PHE:N	2.73	0.41
1:A:65:LYS:O	1:A:69:PRO:HB3	2.21	0.41
2:B:281:PRO:HG2	2:B:306:ILE:HB	2.03	0.41
2:B:281:PRO:HB3	2:B:337:PHE:HB3	2.01	0.41
3:C:8:DG:H2"	3:C:9:DG:H8	1.86	0.41
1:A:37:PHE:CD1	1:A:40:SER:HB3	2.55	0.41
1:A:89:MET:HE3	1:A:107:ALA:HB2	2.01	0.41
1:A:195:LYS:CE	1:A:200:ASN:HA	2.50	0.41
2:B:105:ASP:O	2:B:106:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:219:GLU:N	7:F:2005:HOH:O	2.52	0.41
1:A:134:GLU:O	1:A:134:GLU:HG2	2.20	0.41
1:A:157:MET:HE3	1:A:166:ILE:HD11	2.02	0.41
2:B:8:PHE:N	2:B:8:PHE:CD1	2.89	0.41
2:B:9:ASP:OD1	2:B:160:PRO:HA	2.21	0.41
2:B:239:THR:O	2:B:240:ARG:HB3	2.21	0.41
1:A:161:ASN:O	1:A:161:ASN:CG	2.59	0.41
1:A:250:THR:HG23	1:A:332:ARG:HD2	2.03	0.41
2:B:167:ASP:OD1	2:B:169:GLU:HB3	2.20	0.41
2:B:311:ALA:C	2:B:313:SER:N	2.74	0.41
1:A:173:ARG:NH1	1:A:173:ARG:CB	2.84	0.41
1:A:201:LYS:O	1:A:202:LEU:C	2.60	0.41
2:B:136:GLU:OE1	2:B:136:GLU:HA	2.21	0.41
2:B:196:LYS:C	2:B:198:GLY:N	2.72	0.41
2:B:205:THR:O	2:B:207:SER:N	2.54	0.41
2:B:214:LYS:O	2:B:214:LYS:HG2	2.20	0.41
2:B:248:ILE:HD11	7:B:2035:HOH:O	2.20	0.41
1:A:116:ARG:HD2	1:A:116:ARG:HA	1.90	0.41
1:A:118:TYR:C	1:A:120:GLU:N	2.73	0.41
1:A:166:ILE:CG2	1:A:170:GLU:HB3	2.51	0.41
1:A:181:ALA:HA	1:A:186:ILE:CG2	2.50	0.41
2:B:11:PHE:CE2	2:B:104:ILE:HG12	2.54	0.41
1:A:308:LYS:HB2	1:A:308:LYS:HE3	1.86	0.40
2:B:19:LEU:HD21	2:B:80:VAL:HG11	2.03	0.40
2:B:111:ILE:CD1	2:B:111:ILE:N	2.71	0.40
2:B:139:THR:CG2	2:B:161:ASN:ND2	2.85	0.40
1:A:9:ASP:C	1:A:11:PHE:N	2.72	0.40
1:A:331:ARG:NH1	4:E:5:O2G:P	2.84	0.40
2:B:7:ASP:OD1	2:B:106:GLU:HG2	2.21	0.40
2:B:174:LEU:O	2:B:175:ILE:C	2.59	0.40
4:F:13:DT:H2'	4:F:14:DC:H6	1.86	0.40
2:B:122:TYR:O	2:B:126:LEU:HD12	2.21	0.40
2:B:256:ARG:O	2:B:256:ARG:HG3	2.21	0.40
2:B:259:GLU:HA	2:B:262:LYS:HG2	2.02	0.40
2:B:171:VAL:O	2:B:171:VAL:HG12	2.21	0.40
2:B:281:PRO:O	2:B:306:ILE:N	2.54	0.40
2:B:298:ARG:HA	2:B:298:ARG:HD3	1.79	0.40
1:A:20:ASN:HD22	1:A:23:LEU:HG	1.85	0.40
1:A:21:PRO:C	1:A:23:LEU:N	2.74	0.40
1:A:135:LYS:HE2	1:A:135:LYS:HB3	1.97	0.40
2:B:202:LEU:HD21	2:B:228:LEU:CB	2.51	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:176:ARG:NH1	4:F:3:DA:O5'[2_656]	1.90	0.30

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	340/358 (95%)	271 (80%)	46 (14%)	23 (7%)	1 3
2	B	340/358 (95%)	259 (76%)	63 (18%)	18 (5%)	2 6
All	All	680/716 (95%)	530 (78%)	109 (16%)	41 (6%)	1 4

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASN
1	A	96	SER
1	A	111	ILE
1	A	202	LEU
1	A	203	VAL
1	A	234	ASN
1	A	240	ARG
1	A	258	LEU
1	A	277	ASP
2	B	8	PHE
2	B	115	VAL
2	B	234	ASN
2	B	254	ASN
2	B	255	SER
2	B	258	LEU
1	A	10	TYR
1	A	24	LYS

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Mol	Chain	Res	Type
1	A	36	ARG
1	A	52	LYS
1	A	233	TYR
1	A	239	THR
1	A	300	ARG
2	B	112	SER
2	B	259	GLU
2	B	262	LYS
2	B	277	ASP
1	A	110	ASP
1	A	117	ASP
1	A	214	LYS
2	B	90	ASN
2	B	208	ILE
2	B	233	TYR
2	B	260	GLU
1	A	11	PHE
1	A	244	SER
2	B	69	PRO
2	B	240	ARG
1	A	167	ASP
1	A	271	GLU
2	B	146	LYS
2	B	27	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	300/315 (95%)	267 (89%)	33 (11%)	6 19
2	B	300/315 (95%)	255 (85%)	45 (15%)	3 9
All	All	600/630 (95%)	522 (87%)	78 (13%)	4 12

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	A	49	GLU
1	A	63	GLU
1	A	91	LEU
1	A	97	GLU
1	A	98	LYS
1	A	117	ASP
1	A	127	GLU
1	A	167	ASP
1	A	168	ASP
1	A	169	GLU
1	A	172	LYS
1	A	195	LYS
1	A	197	LEU
1	A	202	LEU
1	A	205	THR
1	A	207	SER
1	A	208	ILE
1	A	211	ASP
1	A	216	MET
1	A	235	GLU
1	A	238	ARG
1	A	241	VAL
1	A	250	THR
1	A	252	LYS
1	A	253	ARG
1	A	270	GLU
1	A	280	ILE
1	A	291	GLU
1	A	295	ILE
1	A	327	GLU
1	A	328	ARG
1	A	336	ARG
2	B	24	LYS
2	B	45	THR
2	B	51	ARG
2	B	63	GLU
2	B	66	LYS
2	B	76	MET
2	B	79	GLU
2	B	82	GLN
2	B	83	GLN
2	B	111	ILE

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Mol	Chain	Res	Type
2	B	119	ARG
2	B	124	LEU
2	B	132	ILE
2	B	134	GLU
2	B	146	LYS
2	B	147	ASN
2	B	168	ASP
2	B	180	ILE
2	B	188	ASN
2	B	202	LEU
2	B	207	SER
2	B	212	LYS
2	B	214	LYS
2	B	240	ARG
2	B	252	LYS
2	B	253	ARG
2	B	256	ARG
2	B	272	SER
2	B	273	TYR
2	B	274	TYR
2	B	276	LEU
2	B	277	ASP
2	B	284	ILE
2	B	292	ASP
2	B	293	LEU
2	B	295	ILE
2	B	296	VAL
2	B	301	THR
2	B	320	GLN
2	B	324	GLU
2	B	328	ARG
2	B	329	LYS
2	B	332	ARG
2	B	336	ARG
2	B	340	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	ASN
2	B	82	GLN
2	B	320	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	O2G	E	5	4	20,26,27	1.28	2 (10%)	22,38,41	2.14	5 (22%)
3	DOC	D	13	3,4	16,19,20	3.28	4 (25%)	20,26,29	4.67	4 (20%)
4	O2G	F	5	4	20,26,27	1.34	2 (10%)	22,38,41	1.87	6 (27%)
3	DOC	C	13	3,4	16,19,20	3.24	4 (25%)	20,26,29	4.43	5 (25%)

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	O2G	E	5	4	-	2/7/25/26	0/3/3/3
3	DOC	D	13	3,4	-	1/7/18/19	0/2/2/2
4	O2G	F	5	4	-	0/7/25/26	0/3/3/3
3	DOC	C	13	3,4	-	2/7/18/19	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	DOC	O4'-C4'	-10.97	1.22	1.44
3	D	13	DOC	O4'-C4'	-10.76	1.23	1.44
3	C	13	DOC	C3'-C2'	4.85	1.67	1.54
3	D	13	DOC	C3'-C2'	4.44	1.66	1.54
3	D	13	DOC	C5'-C4'	3.78	1.62	1.50
4	F	5	O2G	C5-C6	-3.65	1.40	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	13	DOC	O5'-C5'	3.55	1.53	1.44
4	E	5	O2G	C5-C6	-3.20	1.40	1.47
4	F	5	O2G	C2-N3	3.09	1.34	1.30
3	C	13	DOC	O5'-C5'	3.05	1.52	1.44
4	E	5	O2G	C2-N3	2.91	1.34	1.30
3	C	13	DOC	C5'-C4'	2.90	1.59	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	13	DOC	O4'-C4'-C5'	16.53	136.71	109.52
3	C	13	DOC	O4'-C4'-C5'	15.18	134.48	109.52
3	C	13	DOC	O4'-C4'-C3'	8.88	119.53	104.80
3	D	13	DOC	O4'-C4'-C3'	8.60	119.07	104.80
3	D	13	DOC	C2'-C3'-C4'	-7.16	89.31	102.72
3	C	13	DOC	C2'-C3'-C4'	-6.76	90.06	102.72
4	E	5	O2G	N1-C2-N2	6.73	123.77	118.04
4	F	5	O2G	N1-C2-N2	5.49	122.71	118.04
3	C	13	DOC	C2'-C1'-N1	4.98	121.85	112.40
3	D	13	DOC	O4'-C1'-N1	4.89	116.61	107.86
4	E	5	O2G	C2'-C1'-N9	-4.46	103.97	114.27
4	F	5	O2G	C8-N7-C5	2.81	108.35	102.99
4	E	5	O2G	C8-N7-C5	2.79	108.31	102.99
4	F	5	O2G	C5-C6-N1	2.70	118.73	113.95
3	C	13	DOC	O4'-C1'-N1	2.64	112.59	107.86
4	E	5	O2G	C5-C6-N1	2.46	118.29	113.95
4	F	5	O2G	C2-N1-C6	-2.44	119.67	123.71
4	F	5	O2G	O6-C6-C5	-2.37	119.73	124.37
4	F	5	O2G	O4'-C4'-C5'	-2.15	102.31	109.37
4	E	5	O2G	O6-C6-C5	-2.11	120.24	124.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	5	O2G	O4'-C4'-C5'-O5'
4	E	5	O2G	C3'-C4'-C5'-O5'
3	C	13	DOC	C3'-C4'-C5'-O5'
3	D	13	DOC	C3'-C4'-C5'-O5'
3	C	13	DOC	O4'-C1'-N1-C6

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	5	O2G	11	0
3	D	13	DOC	1	0
4	F	5	O2G	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	TTP	B	1345	5	26,30,30	1.68	5 (19%)	39,47,47	2.56	12 (30%)
6	TTP	A	1345	5	26,30,30	1.90	7 (26%)	39,47,47	2.81	14 (35%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	TTP	B	1345	5	-	5/22/34/34	0/2/2/2
6	TTP	A	1345	5	-	3/22/34/34	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1345	TTP	C6-C5	4.60	1.42	1.34
6	B	1345	TTP	C4-C5	-3.99	1.38	1.44
6	B	1345	TTP	PG-O1G	3.81	1.62	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1345	TTP	PG-O1G	3.47	1.61	1.50
6	B	1345	TTP	C6-C5	3.42	1.40	1.34
6	A	1345	TTP	C4-C5	-3.32	1.39	1.44
6	A	1345	TTP	C1'-N1	-3.13	1.40	1.48
6	A	1345	TTP	PA-O1A	3.00	1.61	1.50
6	A	1345	TTP	PB-O1B	2.95	1.61	1.50
6	B	1345	TTP	PB-O1B	2.56	1.60	1.50
6	A	1345	TTP	C2-N3	2.38	1.42	1.38
6	B	1345	TTP	PA-O1A	2.30	1.59	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1345	TTP	C5-C4-N3	7.89	122.05	115.31
6	A	1345	TTP	C5-C4-N3	7.46	121.68	115.31
6	A	1345	TTP	C4-N3-C2	-6.79	118.56	127.35
6	B	1345	TTP	C4-N3-C2	-6.22	119.30	127.35
6	A	1345	TTP	O4'-C1'-N1	-5.92	97.28	107.86
6	B	1345	TTP	PB-O3B-PG	-5.13	115.21	132.83
6	A	1345	TTP	C2'-C1'-N1	-5.13	101.96	113.77
6	A	1345	TTP	O4-C4-C5	-4.99	119.12	124.90
6	A	1345	TTP	PB-O3B-PG	-4.86	116.15	132.83
6	A	1345	TTP	PB-O3A-PA	-4.79	116.40	132.83
6	B	1345	TTP	PB-O3A-PA	-4.76	116.50	132.83
6	A	1345	TTP	N3-C2-N1	4.70	121.13	114.89
6	B	1345	TTP	O4-C4-C5	-4.48	119.71	124.90
6	B	1345	TTP	C2'-C1'-N1	-4.23	104.04	113.77
6	B	1345	TTP	C5-C6-N1	-3.97	119.25	123.34
6	A	1345	TTP	O3G-PG-O3B	2.81	114.07	104.64
6	B	1345	TTP	N3-C2-N1	2.73	118.51	114.89
6	B	1345	TTP	O3G-PG-O3B	2.62	113.41	104.64
6	B	1345	TTP	C5M-C5-C6	-2.48	119.54	122.85
6	A	1345	TTP	C5M-C5-C4	2.43	121.45	118.77
6	B	1345	TTP	C5M-C5-C4	2.35	121.36	118.77
6	A	1345	TTP	C5-C6-N1	-2.32	120.95	123.34
6	A	1345	TTP	O2-C2-N1	-2.31	119.71	122.79
6	A	1345	TTP	C6-N1-C2	-2.29	118.98	121.30
6	A	1345	TTP	C5M-C5-C6	-2.24	119.86	122.85
6	B	1345	TTP	O2-C2-N1	-2.12	119.97	122.79

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1345	TTP	C5'-O5'-PA-O3A
6	B	1345	TTP	C5'-O5'-PA-O3A
6	B	1345	TTP	PG-O3B-PB-O1B
6	A	1345	TTP	C5'-O5'-PA-O1A
6	B	1345	TTP	C5'-O5'-PA-O1A
6	B	1345	TTP	PB-O3B-PG-O3G
6	A	1345	TTP	O4'-C4'-C5'-O5'
6	B	1345	TTP	O4'-C4'-C5'-O5'

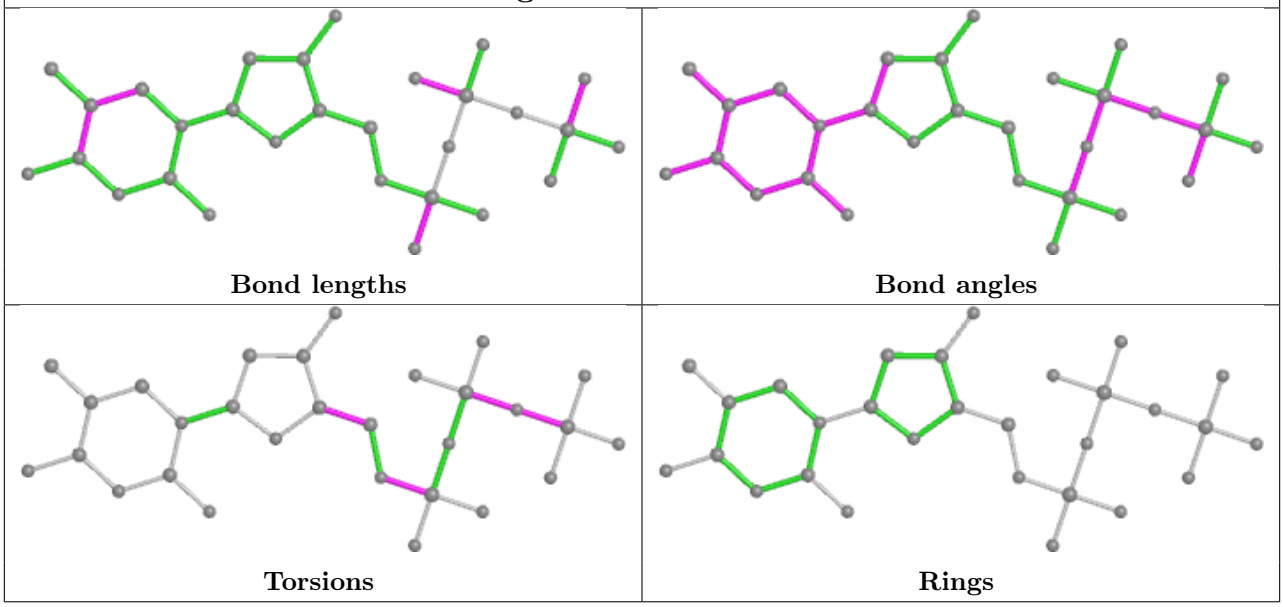
There are no ring outliers.

2 monomers are involved in 9 short contacts:

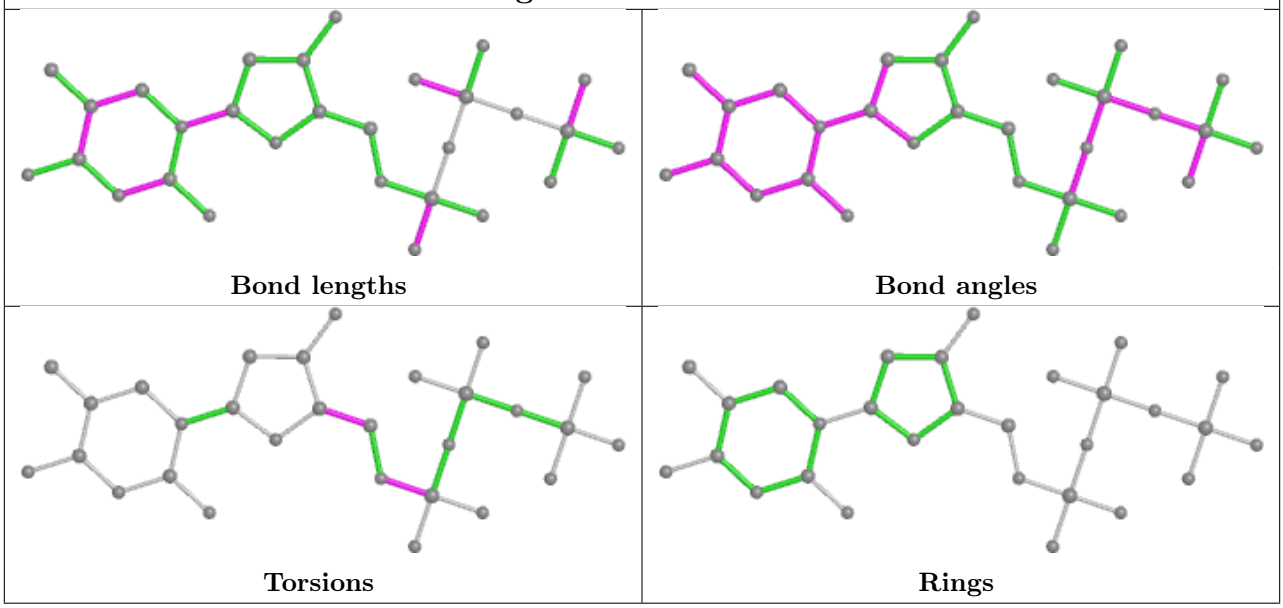
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1345	TTP	4	0
6	A	1345	TTP	5	0

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

Ligand TTP B 1345



Ligand TTP A 1345



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	342/358 (95%)	0.12	1 (0%)	94	94	23, 50, 63, 69	0
2	B	342/358 (95%)	0.12	2 (0%)	89	89	30, 53, 67, 74	0
3	C	12/13 (92%)	-0.31	0	100	100	44, 50, 55, 57	0
3	D	12/13 (92%)	-0.36	0	100	100	37, 52, 66, 74	0
4	E	15/18 (83%)	-0.13	0	100	100	42, 53, 90, 94	0
4	F	15/18 (83%)	-0.05	0	100	100	35, 53, 71, 88	0
All	All	738/778 (94%)	0.10	3 (0%)	92	93	23, 51, 65, 94	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	249	VAL	3.0
1	A	77	ARG	2.2
2	B	253	ARG	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	O2G	E	5	24/25	0.92	0.17	35,42,81,82	0
3	DOC	D	13	18/19	0.93	0.20	45,51,52,53	0
4	O2G	F	5	24/25	0.93	0.22	42,49,56,58	0
3	DOC	C	13	18/19	0.94	0.20	47,51,55,56	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

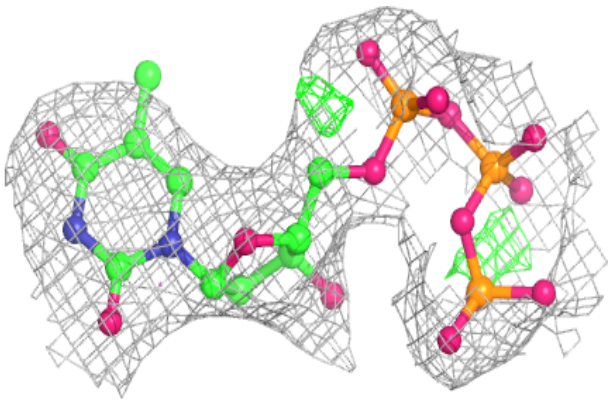
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

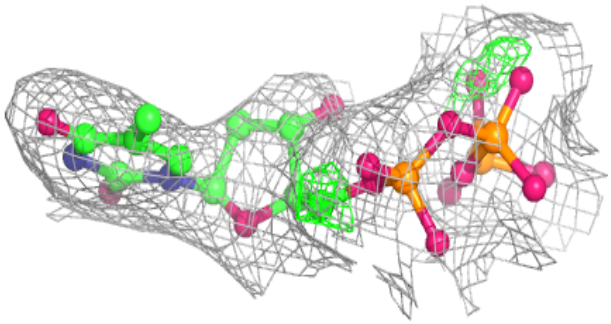
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	B	1342	1/1	0.73	0.10	67,67,67,67	0
5	MG	A	1344	1/1	0.92	0.14	76,76,76,76	0
6	TTP	A	1345	29/29	0.92	0.19	52,57,64,65	0
5	MG	B	1344	1/1	0.93	0.26	56,56,56,56	0
6	TTP	B	1345	29/29	0.93	0.18	31,61,81,86	0
5	MG	A	1342	1/1	0.94	0.18	68,68,68,68	0
5	MG	B	1343	1/1	0.95	0.11	44,44,44,44	0
5	MG	A	1343	1/1	0.96	0.13	25,25,25,25	0

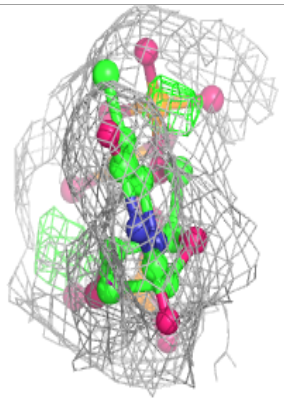
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TTP A 1345:

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

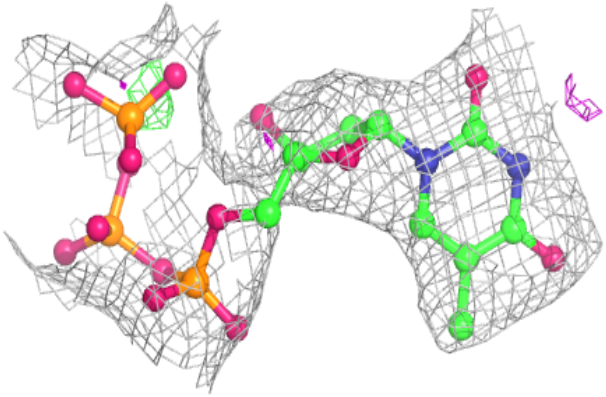


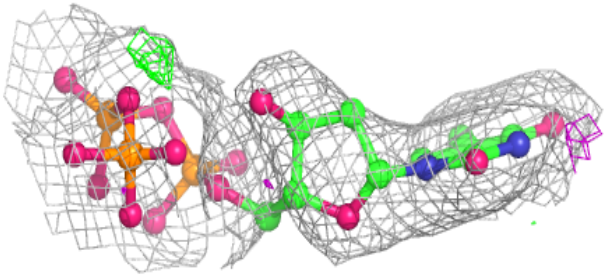


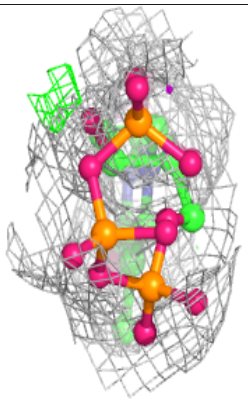


Electron density around TTP B 1345:

$2mF_o$-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.