



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:53 PM UTC

PDB ID : 2W7O / pdb_00002w7o
Title : Structure and Activity of Bypass Synthesis by Human DNA Polymerase Kappa
Opposite the 7,8-Dihydro-8-oxodeoxyguanosine Adduct
Authors : Irimia, A.; Egli, M.
Deposited on : 2008-12-23
Resolution : 3.16 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

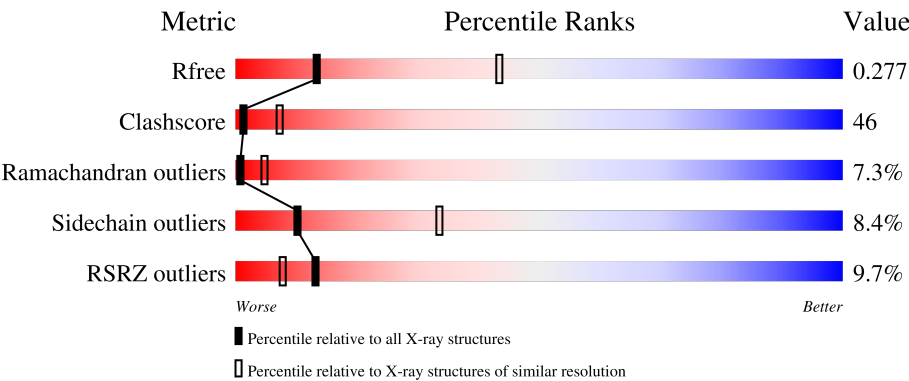
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 3.16 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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 $\leq 5\%$. 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	508	6% 31% 44% 9% 15%
1	B	508	10% 23% 48% 12% 15%
2	E	13	15% 8% 77% 15%
2	P	13	15% 15% 85%
3	F	18	22% 22% 56% 6% 17%

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Mol	Chain	Length	Quality of chain
3	T	18	11% 11% 61% 22% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8136 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 KAPPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	432	Total	C	N	O	S	0	0	1
			3461	2181	614	645	21			
1	B	430	Total	C	N	O	S	0	0	1
			3443	2170	610	642	21			

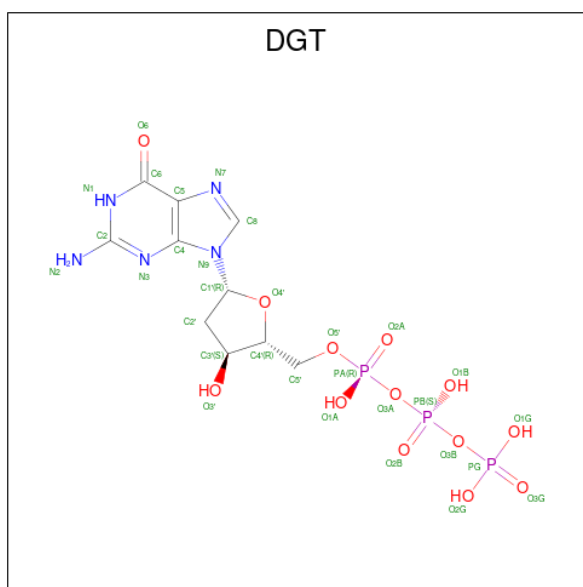
- Molecule 2 is a DNA chain called 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	11	Total	C	N	O	P	0	0	0
			229	109	47	63	10			
2	P	13	Total	C	N	O	P	0	0	0
			273	129	57	75	12			

- Molecule 3 is a DNA chain called 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP*TP*CP*CP*CP*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	15	Total	C	N	O	P	0	0	0
			298	143	52	89	14			
3	T	17	Total	C	N	O	P	0	0	0
			336	161	58	101	16			

- Molecule 4 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	2	Total	Ca	0	0
			2	2		

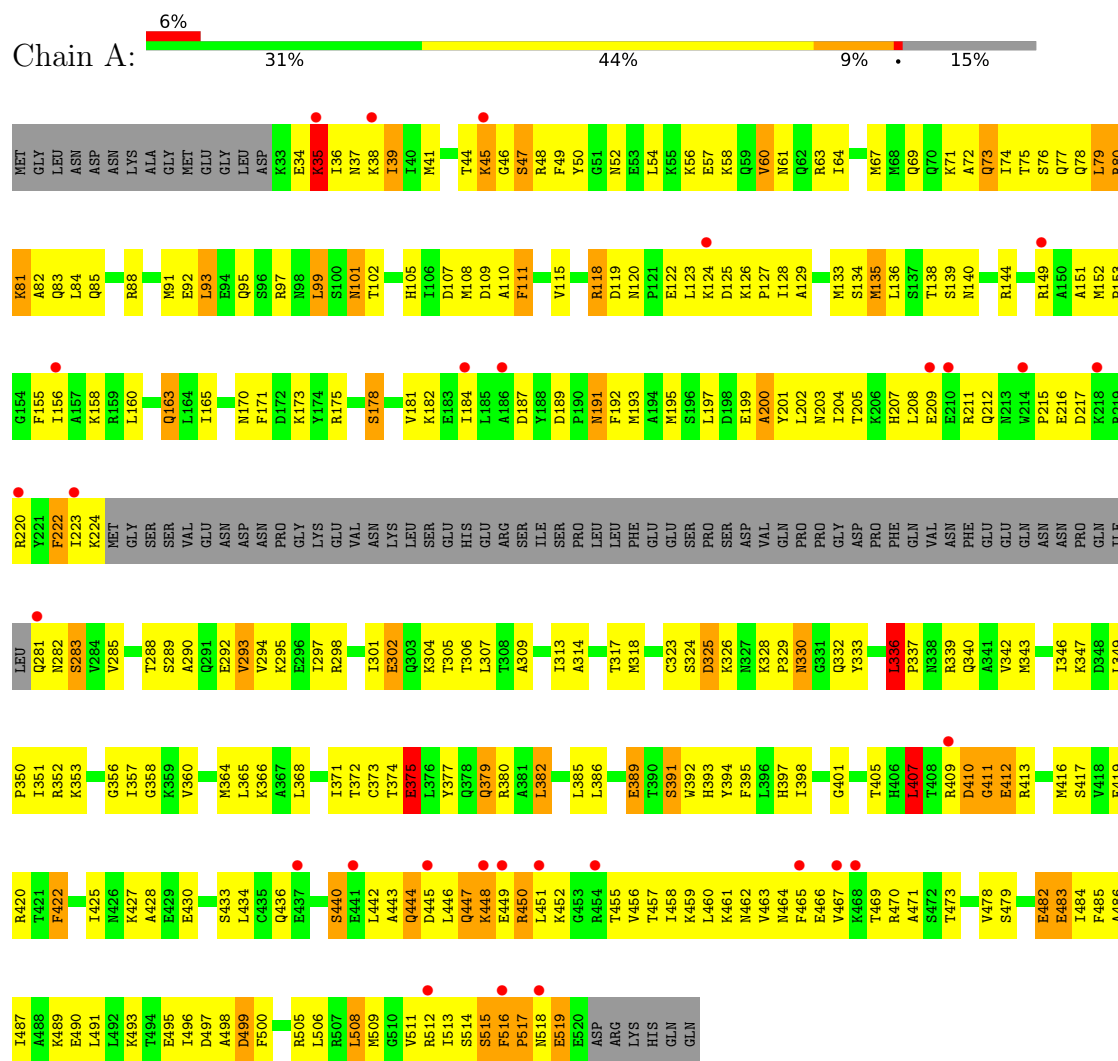
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	6	Total	O	0	0
			6	6		
6	P	2	Total	O	0	0
			2	2		
6	T	1	Total	O	0	0
			1	1		

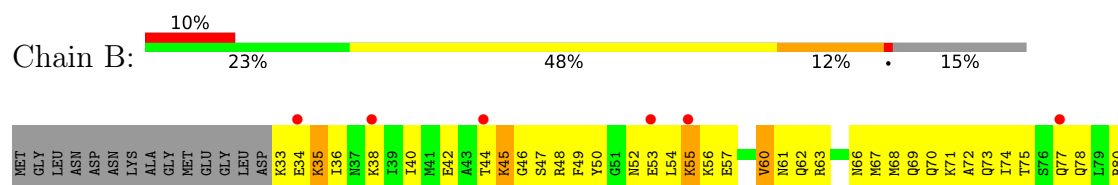
3 Residue-property plots

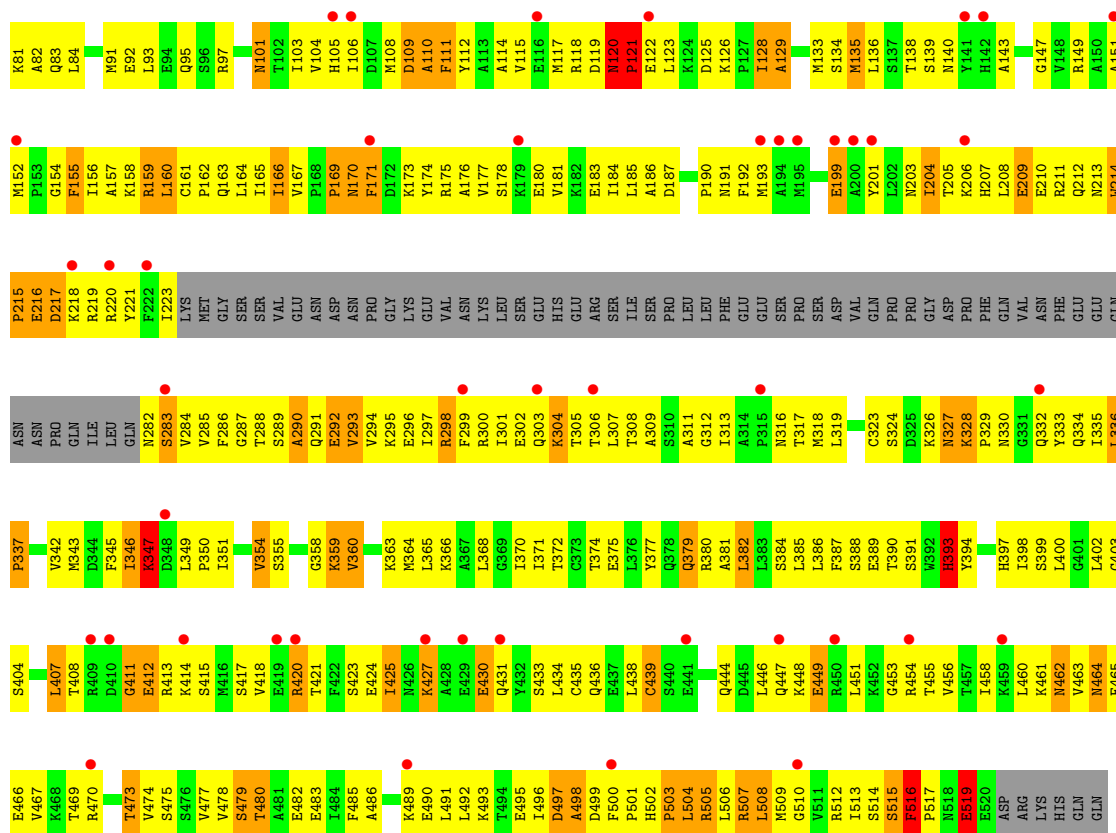
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 KAPPA

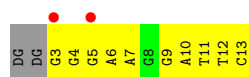


• Molecule 1: DNA POLYMERASE KAPPA

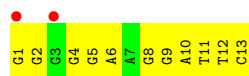




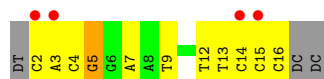
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3'



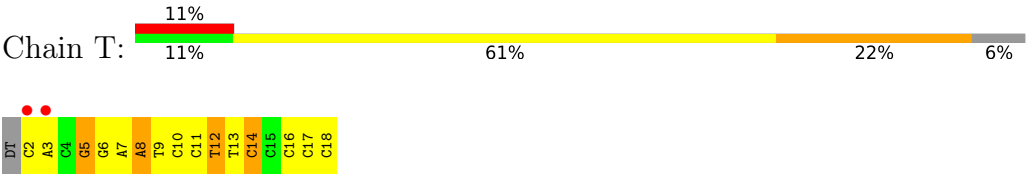
• Molecule 2: 5'-D(*GP*GP*GP*GP*GP*AP*AP*GP*GP*AP*TP*TP*C)-3'



• Molecule 3: 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP* TP*CP*CP*CP*CP*C)-3'



• Molecule 3: 5'-D(TP*CP*AP*CP*8OGP*GP*AP*AP*TP*CP*CP*TP* TP*CP*CP*CP*CP*C)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.48Å 217.63Å 117.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.41 – 3.16 49.41 – 3.16	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.41-3.16) 95.0 (49.41-3.16)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.241 , 0.278 0.234 , 0.277	Depositor DCC
R_{free} test set	1857 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	71.4	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 8OG, CA, DGT

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	0.62	1/3514 (0.0%)	1.04	21/4722 (0.4%)
1	B	0.51	1/3496 (0.0%)	1.01	22/4699 (0.5%)
2	E	0.29	0/258	0.89	0/398
2	P	0.34	0/308	0.97	1/476 (0.2%)
3	F	0.31	0/305	0.91	0/464
3	T	0.38	0/347	1.05	2/528 (0.4%)
All	All	0.54	2/8228 (0.0%)	1.02	46/11287 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	F	0	1
3	T	0	2
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	519	GLU	C-N	-5.63	1.25	1.33
1	B	519	GLU	C-N	-5.37	1.25	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	12	DT	C5'-C4'-C3'	-8.25	102.53	114.90
1	B	295	LYS	N-CA-C	-7.77	102.72	112.90
1	A	393	HIS	N-CA-C	-7.22	103.35	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	ARG	N-CA-C	7.09	119.00	111.28
1	A	48	ARG	N-CA-C	-6.73	103.97	111.71
1	A	35	LYS	N-CA-C	-6.38	104.04	112.72
1	B	360	VAL	N-CA-C	6.31	117.88	111.00
1	A	39	ILE	N-CA-C	-6.28	106.84	112.12
1	B	80	ARG	N-CA-C	-6.20	105.21	112.89
1	A	314	ALA	CA-C-N	6.17	126.06	119.28
1	A	314	ALA	C-N-CA	6.17	126.06	119.28
1	B	35	LYS	N-CA-C	-6.10	105.93	113.19
1	A	417	SER	N-CA-C	6.07	118.19	109.14
1	A	496	ILE	N-CA-C	-6.00	104.67	110.72
1	B	292	GLU	N-CA-C	5.98	117.67	111.03
1	A	440	SER	N-CA-C	-5.98	104.45	110.97
1	B	103	ILE	N-CA-C	5.93	117.73	109.55
1	B	298	ARG	N-CA-C	-5.91	106.07	113.28
1	B	290	ALA	N-CA-C	-5.86	104.80	111.07
1	B	393	HIS	N-CA-C	-5.85	104.91	111.28
1	A	171	PHE	N-CA-C	5.83	117.64	111.28
1	B	449	GLU	N-CA-C	-5.79	103.95	113.50
1	A	407	LEU	N-CA-C	-5.73	101.99	110.48
1	B	501	PRO	N-CA-C	-5.70	107.02	114.03
1	A	178	SER	N-CA-C	-5.69	105.00	111.14
1	A	374	THR	N-CA-C	-5.64	105.05	111.14
1	B	464	ASN	N-CA-C	-5.63	105.72	112.59
1	B	327	ASN	N-CA-C	-5.61	103.86	111.55
1	B	439	CYS	N-CA-C	-5.59	104.56	111.33
1	B	516	PHE	N-CA-C	5.59	122.16	109.81
1	A	336	LEU	CA-C-N	5.58	125.29	119.82
1	A	336	LEU	C-N-CA	5.58	125.29	119.82
1	A	187	ASP	N-CA-C	-5.47	106.56	113.18
1	B	374	THR	N-CA-C	-5.42	105.29	111.14
3	T	14	DC	C5'-C4'-C3'	-5.34	106.90	114.90
2	P	12	DT	C5'-C4'-C3'	-5.31	106.94	114.90
1	B	336	LEU	CA-C-N	5.29	126.46	119.84
1	B	336	LEU	C-N-CA	5.29	126.46	119.84
1	B	209	GLU	N-CA-C	-5.28	105.17	111.03
1	B	159	ARG	N-CA-C	-5.26	106.05	113.20
1	A	448	LYS	N-CA-C	-5.24	105.04	111.75
1	B	507	ARG	N-CA-C	-5.24	106.41	114.16
1	A	58	LYS	N-CA-C	-5.22	105.03	111.40
1	A	375	GLU	N-CA-C	-5.19	105.52	111.07
1	A	175	ARG	N-CA-C	-5.14	105.57	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLU	N-CA-C	5.08	116.79	109.07

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	7	DA	Sidechain
3	T	6	DG	Sidechain
3	T	8	DA	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	3461	0	3546	288	0
1	B	3443	0	3525	393	0
2	E	229	0	125	20	0
2	P	273	0	147	10	0
3	F	298	0	170	19	0
3	T	336	0	192	16	0
4	A	31	0	12	6	0
4	B	31	0	12	5	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	21	0	0	3	0
6	B	6	0	0	0	0
6	P	2	0	0	0	0
6	T	1	0	0	0	0
All	All	8136	0	7729	733	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 46.

All (733) 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:B:502:HIS:HB2	1:B:503:PRO:HD2	1.30	1.12
1:B:128:ILE:HG12	1:B:140:ASN:HD22	1.17	1.10
1:B:453:GLY:HA2	1:B:516:PHE:HB3	1.14	1.09
1:B:118:ARG:HH11	1:B:306:THR:HG22	1.15	1.06
3:F:14:DC:H2''	3:F:15:DC:H5''	1.38	1.05
1:B:108:MET:HA	1:B:309:ALA:HA	1.40	1.04
1:A:128:ILE:H	1:A:140:ASN:ND2	1.56	1.02
1:B:478:VAL:HG13	1:B:483:GLU:HB3	1.47	0.96
3:T:12:DT:H2''	3:T:13:DT:H5'	1.47	0.94
1:A:478:VAL:HG13	1:A:483:GLU:HB2	1.45	0.94
1:B:301:ILE:O	1:B:305:THR:HG22	1.68	0.93
1:B:203:ASN:HB2	1:B:407:LEU:HD11	1.51	0.90
1:B:180:GLU:HG2	1:B:304:LYS:HE3	1.52	0.89
1:B:118:ARG:NH1	1:B:306:THR:HG22	1.87	0.88
1:A:455:THR:OG1	1:A:473:THR:HG22	1.75	0.87
1:B:407:LEU:HD12	1:B:407:LEU:H	1.40	0.86
1:B:121:PRO:O	1:B:122:GLU:HB3	1.75	0.86
1:A:80:ARG:HH11	1:A:80:ARG:HB3	1.41	0.85
1:B:171:PHE:HB3	1:B:175:ARG:HH21	1.41	0.84
1:B:155:PHE:HD2	1:B:156:ILE:H	1.25	0.84
2:P:1:DG:HO5'	2:P:1:DG:H8	1.26	0.83
3:F:4:DC:H6	3:F:4:DC:H5'	1.44	0.83
1:B:328:LYS:HB3	1:B:329:PRO:HD3	1.62	0.82
1:A:101:ASN:HD22	1:A:101:ASN:H	1.27	0.81
1:A:84:LEU:HB2	1:B:95:GLN:NE2	1.95	0.81
1:A:485:PHE:HE1	1:A:489:LYS:HB3	1.43	0.81
1:B:190:PRO:HG2	1:B:191:ASN:H	1.45	0.80
1:A:330:ASN:C	1:A:330:ASN:HD22	1.89	0.80
1:B:203:ASN:HD21	1:B:205:THR:HB	1.46	0.80
4:B:1520:DGT:H5'A	4:B:1520:DGT:PB	2.21	0.80
1:B:192:PHE:HD1	1:B:193:MET:N	1.80	0.80
1:A:208:LEU:HD11	1:A:290:ALA:HB2	1.64	0.79
1:B:101:ASN:N	1:B:101:ASN:HD22	1.78	0.79
1:B:431:GLN:NE2	1:B:506:LEU:HD13	1.98	0.78
2:P:4:DG:H2''	2:P:5:DG:H5''	1.64	0.78
1:A:163:GLN:HB3	6:A:2005:HOH:O	1.84	0.76
1:A:107:ASP:CG	1:A:328:LYS:HZ3	1.93	0.76
1:A:485:PHE:CE1	1:A:489:LYS:HB3	2.21	0.76
1:A:44:THR:HG22	1:A:50:TYR:HB2	1.67	0.76
1:B:223:ILE:HD12	1:B:282:ASN:HA	1.68	0.76
1:A:128:ILE:HG13	1:A:140:ASN:HD22	1.49	0.76
1:B:334:GLN:HG2	1:B:335:ILE:H	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ILE:H	1:A:140:ASN:HD21	1.33	0.76
1:B:214:TRP:N	1:B:215:PRO:HD3	2.01	0.76
1:B:44:THR:HG23	3:F:4:DC:N4	2.00	0.76
1:B:83:GLN:NE2	1:B:381:ALA:HB2	2.01	0.75
2:E:5:DG:H2''	2:E:6:DA:C8	2.21	0.75
1:A:304:LYS:O	1:A:304:LYS:HG2	1.85	0.75
1:A:34:GLU:OE2	1:A:34:GLU:HA	1.87	0.74
3:F:14:DC:C2'	3:F:15:DC:H5''	2.16	0.74
1:B:128:ILE:HG12	1:B:140:ASN:ND2	1.99	0.74
1:B:508:LEU:HD13	1:B:509:MET:N	2.03	0.74
1:A:149:ARG:HG2	1:A:152:MET:HE3	1.70	0.74
1:B:313:ILE:HB	1:B:334:GLN:HG3	1.70	0.74
1:B:328:LYS:HE2	1:B:328:LYS:HA	1.70	0.74
1:A:462:ASN:ND2	1:A:464:ASN:HB2	2.03	0.74
1:A:75:THR:H	1:A:78:GLN:NE2	1.86	0.74
1:B:155:PHE:HB2	1:B:159:ARG:NH1	2.03	0.73
1:B:62:GLN:O	1:B:66:ASN:HB2	1.88	0.73
1:B:359:LYS:HG3	1:B:360:VAL:H	1.52	0.73
1:A:449:GLU:O	1:A:451:LEU:HG	1.88	0.73
1:B:44:THR:HG23	3:F:4:DC:H42	1.50	0.73
1:B:427:LYS:HB2	1:B:430:GLU:HB3	1.70	0.73
2:E:4:DG:H1'	2:E:5:DG:H5''	1.69	0.73
1:A:351:ILE:HG13	1:A:357:ILE:HG21	1.71	0.72
1:A:457:THR:HA	1:A:471:ALA:HB2	1.71	0.72
1:B:129:ALA:HB1	1:B:136:LEU:HD22	1.70	0.72
1:B:135:MET:HE2	1:B:135:MET:HA	1.71	0.72
1:B:53:GLU:O	1:B:57:GLU:HG3	1.89	0.72
1:B:421:THR:OG1	1:B:508:LEU:HD23	1.90	0.71
1:B:97:ARG:HH21	1:B:402:LEU:CD2	2.04	0.71
1:B:214:TRP:N	1:B:215:PRO:CD	2.54	0.71
1:A:101:ASN:HD22	1:A:101:ASN:N	1.88	0.71
1:B:135:MET:HE2	1:B:136:LEU:H	1.55	0.71
1:B:293:VAL:O	1:B:297:ILE:HG13	1.91	0.71
1:B:413:ARG:HD3	1:B:415:SER:O	1.90	0.71
1:A:97:ARG:HG2	1:A:99:LEU:CD1	2.19	0.71
1:B:381:ALA:O	1:B:384:SER:HB3	1.89	0.71
1:B:412:GLU:OE1	1:B:517:PRO:HB3	1.91	0.71
3:F:2:DC:H2'	3:F:2:DC:O2	1.89	0.71
1:B:54:LEU:C	1:B:56:LYS:H	1.98	0.71
1:B:504:LEU:HD22	1:B:506:LEU:HD12	1.73	0.70
1:B:171:PHE:CB	1:B:175:ARG:HH21	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:LEU:HD22	1:A:509:MET:N	2.05	0.70
1:B:480:THR:HG23	1:B:483:GLU:OE1	1.91	0.70
3:F:2:DC:H2''	3:F:3:DA:H8	1.56	0.70
1:A:427:LYS:O	1:A:430:GLU:HB2	1.90	0.70
1:B:109:ASP:HA	4:B:1520:DGT:O1G	1.92	0.70
1:B:110:ALA:HB3	1:B:114:ALA:HB2	1.74	0.70
1:B:289:SER:OG	1:B:292:GLU:HB2	1.92	0.70
1:B:502:HIS:HB2	1:B:503:PRO:CD	2.17	0.70
1:A:128:ILE:H	1:A:140:ASN:HD22	1.38	0.69
1:A:91:MET:HE1	1:B:91:MET:HE1	1.73	0.69
1:B:115:VAL:HG22	1:B:307:LEU:HD11	1.74	0.69
1:B:417:SER:HB3	1:B:512:ARG:HG3	1.74	0.69
1:A:50:TYR:CE1	1:A:54:LEU:HD21	2.28	0.69
1:B:316:ASN:HD21	1:B:319:LEU:H	1.40	0.69
1:A:318:MET:HE2	1:A:398:ILE:HA	1.74	0.69
1:A:446:LEU:HD11	1:A:513:ILE:HG21	1.73	0.69
3:F:13:DT:H2''	3:F:14:DC:O5'	1.93	0.69
1:A:74:ILE:HA	1:A:78:GLN:HE22	1.57	0.68
3:T:7:DA:H2''	3:T:8:DA:H5'	1.74	0.68
1:A:462:ASN:HD21	1:A:464:ASN:HB2	1.58	0.68
1:A:97:ARG:HG2	1:A:99:LEU:HD13	1.73	0.68
1:A:119:ASP:OD1	1:A:173:LYS:HD3	1.94	0.68
1:B:387:PHE:HB3	1:B:391:SER:HB2	1.76	0.68
1:B:461:LYS:HB3	1:B:508:LEU:HB3	1.75	0.68
1:A:340:GLN:HA	1:A:340:GLN:NE2	2.07	0.68
1:B:158:LYS:HD3	1:B:164:LEU:HB3	1.74	0.68
1:B:502:HIS:CB	1:B:503:PRO:HD2	2.14	0.68
1:B:203:ASN:ND2	1:B:205:THR:HB	2.08	0.68
1:B:454:ARG:HB2	1:B:474:VAL:O	1.94	0.68
1:B:118:ARG:HD3	1:B:306:THR:CG2	2.23	0.67
1:A:478:VAL:CG1	1:A:483:GLU:HB2	2.24	0.67
1:B:192:PHE:CD1	1:B:193:MET:N	2.61	0.67
1:A:391:SER:O	1:A:394:TYR:HB3	1.95	0.67
1:B:35:LYS:O	1:B:38:LYS:HB3	1.94	0.67
1:B:78:GLN:O	1:B:81:LYS:HB3	1.95	0.67
1:B:334:GLN:HG2	1:B:335:ILE:N	2.07	0.67
1:A:135:MET:HA	1:A:153:PRO:HA	1.77	0.67
1:B:121:PRO:C	1:B:123:LEU:H	2.03	0.66
1:B:128:ILE:HG13	1:B:129:ALA:N	2.11	0.66
1:A:74:ILE:HG23	1:A:78:GLN:HE21	1.61	0.66
1:A:101:ASN:N	1:A:101:ASN:ND2	2.44	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:HG3	1:B:162:PRO:HA	1.77	0.66
1:B:519:GLU:H	1:B:519:GLU:CD	2.03	0.66
1:B:317:THR:HG23	1:B:404:SER:O	1.96	0.66
1:B:173:LYS:O	1:B:177:VAL:HG23	1.95	0.66
1:B:485:PHE:CE2	1:B:489:LYS:HD3	2.31	0.66
1:B:118:ARG:HD3	1:B:306:THR:HG22	1.78	0.66
1:A:80:ARG:HB3	1:A:80:ARG:NH1	2.11	0.65
1:A:433:SER:O	1:A:436:GLN:HB3	1.96	0.65
1:B:286:PHE:CD1	1:B:296:GLU:HB2	2.32	0.65
1:B:219:ARG:HB3	1:B:219:ARG:HH11	1.62	0.65
1:B:97:ARG:HH21	1:B:402:LEU:HD21	1.62	0.65
1:B:128:ILE:O	1:B:129:ALA:HB2	1.97	0.65
1:B:298:ARG:O	1:B:302:GLU:HB2	1.96	0.65
1:B:308:THR:HB	1:B:330:ASN:HD22	1.61	0.65
1:B:316:ASN:ND2	1:B:319:LEU:H	1.95	0.65
1:B:204:ILE:HG13	1:B:204:ILE:O	1.97	0.65
2:P:4:DG:C2'	2:P:5:DG:H5''	2.26	0.65
1:A:440:SER:O	1:A:444:GLN:HB2	1.96	0.64
1:A:436:GLN:HB2	1:A:485:PHE:HE2	1.61	0.64
1:B:158:LYS:N	1:B:164:LEU:HD22	2.13	0.64
1:A:461:LYS:HB2	1:A:508:LEU:HD12	1.78	0.64
1:B:327:ASN:ND2	1:B:333:TYR:HB2	2.12	0.64
1:B:453:GLY:CA	1:B:516:PHE:HB3	2.09	0.64
1:B:203:ASN:CB	1:B:407:LEU:HD11	2.25	0.64
1:A:290:ALA:HA	1:A:293:VAL:HG13	1.78	0.64
1:A:514:SER:HA	1:A:516:PHE:HE1	1.63	0.64
1:B:83:GLN:HE21	1:B:381:ALA:HB2	1.61	0.64
1:B:97:ARG:NH2	1:B:400:LEU:O	2.30	0.64
1:B:478:VAL:CG1	1:B:483:GLU:HB3	2.27	0.64
1:A:360:VAL:HG12	1:A:364:MET:HE2	1.79	0.64
1:B:359:LYS:HG3	1:B:360:VAL:N	2.12	0.63
1:A:427:LYS:HD3	1:A:430:GLU:OE2	1.98	0.63
1:B:109:ASP:OD2	1:B:329:PRO:HA	1.98	0.63
1:B:453:GLY:HA2	1:B:516:PHE:CB	2.08	0.63
1:A:305:THR:O	1:A:306:THR:HB	1.99	0.62
1:B:171:PHE:HB3	1:B:175:ARG:NH2	2.11	0.62
1:B:291:GLN:HG2	1:B:334:GLN:NE2	2.14	0.62
1:B:475:SER:O	1:B:477:VAL:HG23	1.98	0.62
1:B:155:PHE:HD2	1:B:156:ILE:N	1.97	0.62
1:B:158:LYS:C	1:B:160:LEU:H	2.06	0.62
1:A:201:TYR:CE1	1:A:317:THR:HG23	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:LYS:CD	1:B:467:VAL:HG22	2.30	0.62
1:A:201:TYR:C	1:A:202:LEU:HD12	2.24	0.62
1:A:203:ASN:C	1:A:205:THR:H	2.07	0.62
1:B:135:MET:HG3	3:F:5:8OG:O4'	1.99	0.62
1:A:60:VAL:HG12	1:A:61:ASN:N	2.15	0.62
1:A:216:GLU:HG3	1:A:285:VAL:HG11	1.81	0.62
1:A:461:LYS:HG3	1:A:467:VAL:HG22	1.82	0.62
1:B:213:ASN:C	1:B:215:PRO:HD3	2.24	0.61
1:B:349:LEU:HD23	1:B:349:LEU:C	2.24	0.61
1:B:420:ARG:O	1:B:508:LEU:HD22	2.00	0.61
1:B:431:GLN:HE22	1:B:504:LEU:HB3	1.65	0.61
1:B:492:LEU:HD12	1:B:492:LEU:O	2.00	0.61
1:B:504:LEU:HD22	1:B:506:LEU:CD1	2.29	0.61
1:A:71:LYS:O	1:A:74:ILE:HG13	2.00	0.61
1:A:346:ILE:HD11	1:A:401:GLY:HA3	1.82	0.61
1:B:47:SER:C	1:B:49:PHE:H	2.08	0.61
1:A:95:GLN:NE2	1:B:84:LEU:HB2	2.15	0.61
1:B:504:LEU:HD13	1:B:506:LEU:HD11	1.83	0.61
1:A:81:LYS:HE2	1:A:85:GLN:NE2	2.15	0.61
1:B:33:LYS:O	1:B:36:ILE:HG13	2.01	0.61
1:B:425:ILE:HG22	1:B:425:ILE:O	2.00	0.61
1:B:371:ILE:HG22	1:B:372:THR:HG23	1.83	0.61
1:B:101:ASN:N	1:B:101:ASN:ND2	2.43	0.61
1:B:111:PHE:O	1:B:112:TYR:C	2.43	0.61
1:B:155:PHE:CD2	1:B:156:ILE:N	2.68	0.61
1:B:449:GLU:HB2	1:B:451:LEU:HD23	1.83	0.61
1:B:516:PHE:HD1	1:B:517:PRO:HD3	1.66	0.60
1:A:346:ILE:HG22	1:A:373:CYS:HB2	1.83	0.60
1:A:389:GLU:HA	1:A:392:TRP:CD1	2.37	0.60
1:A:458:ILE:HG22	1:A:470:ARG:O	2.00	0.60
1:A:495:GLU:O	1:A:498:ALA:HB3	2.01	0.60
1:A:410:ASP:O	1:A:412:GLU:N	2.34	0.60
3:F:4:DC:H5'	3:F:4:DC:C6	2.32	0.60
1:B:516:PHE:H	1:B:517:PRO:CD	2.14	0.60
3:F:2:DC:H2''	3:F:3:DA:C8	2.36	0.60
1:B:82:ALA:HB2	1:B:385:LEU:HD21	1.83	0.60
1:A:71:LYS:O	1:A:73:GLN:N	2.33	0.60
1:B:120:ASN:C	1:B:120:ASN:HD22	2.09	0.60
1:B:455:THR:O	1:B:513:ILE:HD12	2.00	0.60
1:B:216:GLU:H	1:B:219:ARG:NH2	2.00	0.59
2:E:5:DG:H2''	2:E:6:DA:N7	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:GLN:HA	1:A:379:GLN:HE21	1.66	0.59
1:B:347:LYS:NZ	1:B:347:LYS:HB3	2.16	0.59
2:E:13:DC:H5'	2:E:13:DC:C6	2.37	0.59
1:A:294:VAL:HG21	1:A:313:ILE:HG12	1.85	0.59
1:A:485:PHE:O	1:A:485:PHE:HD1	1.86	0.59
1:B:211:ARG:O	1:B:211:ARG:HG2	2.00	0.59
1:A:483:GLU:O	1:A:486:ALA:HB3	2.03	0.59
1:B:155:PHE:HB2	1:B:159:ARG:HH12	1.67	0.59
1:A:120:ASN:HD21	1:A:122:GLU:HB3	1.68	0.59
1:A:514:SER:HA	1:A:516:PHE:CE1	2.38	0.59
1:B:45:LYS:HG3	1:B:46:GLY:N	2.17	0.58
1:A:74:ILE:HA	1:A:78:GLN:NE2	2.16	0.58
1:A:506:LEU:CD2	1:A:509:MET:HE3	2.33	0.58
1:B:207:HIS:C	1:B:207:HIS:CD2	2.82	0.58
1:B:516:PHE:H	1:B:517:PRO:HD2	1.68	0.58
1:A:155:PHE:CE1	1:A:156:ILE:HG13	2.38	0.58
1:A:460:LEU:HD22	1:A:506:LEU:HD21	1.85	0.58
1:B:147:GLY:O	1:B:149:ARG:HG2	2.04	0.58
1:B:454:ARG:HG2	1:B:515:SER:O	2.04	0.58
2:E:3:DG:H1	3:F:16:DC:N4	2.01	0.58
1:B:101:ASN:ND2	1:B:101:ASN:H	2.02	0.58
1:B:108:MET:HB3	1:B:308:THR:O	2.04	0.57
1:A:371:ILE:H	1:A:375:GLU:HG3	1.69	0.57
1:B:71:LYS:O	1:B:73:GLN:N	2.37	0.57
1:B:203:ASN:C	1:B:205:THR:H	2.13	0.57
1:B:47:SER:C	1:B:49:PHE:N	2.61	0.57
1:B:482:GLU:CD	1:B:482:GLU:H	2.12	0.57
1:A:215:PRO:C	1:A:217:ASP:H	2.12	0.57
1:B:120:ASN:O	1:B:121:PRO:O	2.23	0.57
1:A:398:ILE:HD12	1:A:398:ILE:H	1.69	0.57
1:A:293:VAL:O	1:A:297:ILE:HG13	2.04	0.57
1:A:328:LYS:HG3	1:A:329:PRO:HA	1.85	0.57
2:P:1:DG:H8	2:P:1:DG:O5'	1.86	0.57
1:A:81:LYS:O	1:A:85:GLN:HG2	2.05	0.56
1:B:138:THR:HG22	1:B:139:SER:N	2.21	0.56
1:B:460:LEU:HD22	1:B:506:LEU:HD21	1.87	0.56
1:A:101:ASN:HB3	1:A:203:ASN:HD21	1.71	0.56
1:B:382:LEU:HD22	1:B:386:LEU:CD1	2.35	0.56
1:A:410:ASP:O	1:A:411:GLY:C	2.48	0.56
1:B:133:MET:C	1:B:154:GLY:HA3	2.30	0.56
1:B:128:ILE:O	1:B:129:ALA:CB	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:O	1:A:386:LEU:HD23	2.05	0.56
1:B:204:ILE:HD12	1:B:293:VAL:HG21	1.86	0.56
1:A:82:ALA:O	1:A:85:GLN:N	2.39	0.56
1:A:305:THR:O	1:A:306:THR:CB	2.54	0.56
1:B:319:LEU:HD11	1:B:342:VAL:HG13	1.86	0.56
2:E:7:DA:H5'	2:E:7:DA:H8	1.71	0.56
1:A:413:ARG:CZ	1:A:416:MET:HE3	2.36	0.55
1:B:463:VAL:HA	1:B:507:ARG:HD2	1.88	0.55
1:A:34:GLU:OE2	1:A:34:GLU:CA	2.55	0.55
1:B:164:LEU:HG	1:B:166:ILE:HG23	1.88	0.55
1:B:304:LYS:HG3	1:B:304:LYS:O	2.06	0.55
1:A:339:ARG:NH2	1:A:343:MET:HE2	2.21	0.55
1:B:120:ASN:H	1:B:121:PRO:HD3	1.72	0.55
1:B:210:GLU:C	1:B:212:GLN:H	2.14	0.55
1:A:76:SER:O	1:A:80:ARG:HG3	2.06	0.55
1:A:366:LYS:HE2	1:A:371:ILE:HD12	1.89	0.55
1:B:97:ARG:NH2	1:B:402:LEU:HD21	2.21	0.55
1:B:297:ILE:O	1:B:301:ILE:HG13	2.07	0.55
1:A:298:ARG:NH1	1:A:332:GLN:OE1	2.41	0.55
1:A:74:ILE:CG2	1:A:78:GLN:HE21	2.20	0.54
1:A:75:THR:N	1:A:78:GLN:NE2	2.54	0.54
1:A:133:MET:HE1	1:A:158:LYS:HZ2	1.72	0.54
1:B:68:MET:O	1:B:71:LYS:HB3	2.07	0.54
1:B:359:LYS:HG3	1:B:360:VAL:HG23	1.89	0.54
1:A:36:ILE:HG23	1:A:160:LEU:HD22	1.89	0.54
1:A:81:LYS:O	1:A:81:LYS:HD3	2.07	0.54
1:A:372:THR:H	1:A:375:GLU:HG3	1.73	0.54
1:B:508:LEU:HD13	1:B:508:LEU:C	2.32	0.54
1:A:44:THR:CG2	1:A:50:TYR:HB2	2.38	0.54
1:A:82:ALA:O	1:A:83:GLN:C	2.50	0.54
1:B:193:MET:HE2	1:B:408:THR:O	2.07	0.54
2:E:3:DG:N2	3:F:16:DC:H42	2.06	0.54
1:A:199:GLU:O	1:A:200:ALA:HB2	2.06	0.54
1:B:34:GLU:C	1:B:36:ILE:H	2.16	0.54
1:B:221:TYR:CE2	1:B:300:ARG:HD2	2.42	0.54
1:A:123:LEU:O	1:A:125:ASP:N	2.41	0.54
1:A:516:PHE:CD1	1:A:516:PHE:N	2.76	0.54
1:B:461:LYS:HG3	1:B:467:VAL:HG22	1.89	0.54
6:A:2020:HOH:O	1:B:343:MET:HE2	2.07	0.54
1:B:106:ILE:O	1:B:199:GLU:HA	2.08	0.54
1:A:63:ARG:CZ	1:A:364:MET:HE1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:C	1:B:56:LYS:N	2.62	0.54
1:B:424:GLU:OE1	1:B:505:ARG:HG2	2.08	0.54
1:A:517:PRO:C	1:A:519:GLU:H	2.16	0.54
1:B:220:ARG:HA	1:B:285:VAL:HA	1.90	0.54
1:A:88:ARG:O	1:A:92:GLU:HG3	2.08	0.53
1:A:382:LEU:HD22	1:A:386:LEU:HG	1.90	0.53
1:B:203:ASN:O	1:B:205:THR:N	2.34	0.53
2:E:4:DG:H2''	2:E:5:DG:C5'	2.37	0.53
1:A:128:ILE:HD12	1:A:129:ALA:N	2.22	0.53
1:B:299:PHE:O	1:B:303:GLN:HG2	2.07	0.53
1:B:470:ARG:HG3	1:B:495:GLU:OE2	2.08	0.53
1:B:477:VAL:HG12	1:B:477:VAL:O	2.07	0.53
2:P:1:DG:H2''	2:P:2:DG:O5'	2.07	0.53
1:A:356:GLY:HA3	1:A:394:TYR:OH	2.08	0.53
1:B:497:ASP:O	1:B:499:ASP:N	2.42	0.53
1:A:46:GLY:O	1:A:47:SER:O	2.26	0.53
1:B:97:ARG:HH21	1:B:402:LEU:HD23	1.73	0.53
1:A:203:ASN:HB2	1:A:407:LEU:HD11	1.90	0.53
1:B:190:PRO:CG	1:B:191:ASN:H	2.19	0.53
1:A:391:SER:HB2	3:T:12:DT:OP1	2.08	0.53
1:B:136:LEU:HD12	1:B:152:MET:O	2.09	0.53
3:T:2:DC:H2''	3:T:3:DA:O5'	2.09	0.53
3:T:12:DT:H2''	3:T:13:DT:C5'	2.32	0.53
1:B:308:THR:CG2	1:B:330:ASN:HD22	2.22	0.52
1:B:412:GLU:HG3	1:B:413:ARG:H	1.74	0.52
1:B:516:PHE:CD1	1:B:517:PRO:HD3	2.44	0.52
2:E:9:DG:H2''	2:E:10:DA:O5'	2.09	0.52
1:A:75:THR:C	1:A:77:GLN:H	2.17	0.52
1:A:105:HIS:NE2	1:A:199:GLU:HG2	2.24	0.52
1:A:223:ILE:HB	1:A:281:GLN:HA	1.92	0.52
1:A:452:LYS:HG2	1:A:479:SER:OG	2.09	0.52
1:B:120:ASN:C	1:B:120:ASN:ND2	2.67	0.52
1:B:136:LEU:HD11	1:B:157:ALA:HB2	1.91	0.52
1:A:419:GLU:HB2	1:A:508:LEU:HD21	1.91	0.52
1:B:82:ALA:O	1:B:83:GLN:C	2.52	0.52
1:B:84:LEU:O	1:B:84:LEU:HD12	2.10	0.52
1:B:169:PRO:O	1:B:170:ASN:HB2	2.10	0.52
1:B:213:ASN:HA	1:B:215:PRO:HD3	1.91	0.52
1:B:294:VAL:HG12	1:B:332:GLN:OE1	2.09	0.52
1:A:192:PHE:O	1:A:201:TYR:O	2.27	0.52
1:B:460:LEU:HD21	1:B:509:MET:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HD3	1:A:165:ILE:HD11	1.92	0.52
1:A:500:PHE:O	1:A:500:PHE:CD2	2.63	0.52
1:B:149:ARG:HG3	1:B:152:MET:HE3	1.92	0.52
1:B:326:LYS:HD3	1:B:333:TYR:CD2	2.44	0.52
1:B:60:VAL:HG12	1:B:61:ASN:N	2.24	0.52
1:B:208:LEU:HD11	1:B:290:ALA:HA	1.90	0.52
1:B:207:HIS:CD2	1:B:211:ARG:HB2	2.44	0.52
1:A:35:LYS:HZ2	1:A:38:LYS:HD3	1.75	0.51
1:A:118:ARG:HD2	1:A:119:ASP:OD2	2.11	0.51
1:A:134:SER:O	1:A:135:MET:HB2	2.09	0.51
1:B:71:LYS:C	1:B:73:GLN:H	2.17	0.51
1:B:506:LEU:CD2	1:B:509:MET:HE3	2.41	0.51
1:A:447:GLN:C	1:A:449:GLU:N	2.65	0.51
1:B:69:GLN:O	1:B:70:GLN:C	2.54	0.51
1:B:109:ASP:O	1:B:111:PHE:N	2.43	0.51
1:B:115:VAL:CG2	1:B:307:LEU:HD11	2.40	0.51
1:B:394:TYR:CZ	1:B:398:ILE:HD11	2.45	0.51
1:A:75:THR:C	1:A:77:GLN:N	2.66	0.51
1:A:457:THR:HA	1:A:471:ALA:CB	2.36	0.51
1:B:48:ARG:HG3	1:B:48:ARG:HH11	1.75	0.51
1:A:84:LEU:HB2	1:B:95:GLN:HE21	1.73	0.51
1:B:216:GLU:O	1:B:217:ASP:O	2.28	0.51
1:A:220:ARG:HB3	1:A:285:VAL:HG22	1.92	0.51
1:B:119:ASP:O	1:B:120:ASN:HB2	2.10	0.51
1:B:287:GLY:H	1:B:292:GLU:HG2	1.74	0.51
1:A:434:LEU:HD13	1:A:434:LEU:C	2.35	0.51
1:B:351:ILE:CD1	1:B:365:LEU:HD12	2.41	0.51
3:T:14:DC:H4'	3:T:14:DC:OP1	2.10	0.51
1:A:346:ILE:O	1:A:347:LYS:C	2.54	0.51
1:B:128:ILE:HG12	1:B:140:ASN:HB2	1.92	0.51
1:B:308:THR:CB	1:B:330:ASN:HD22	2.23	0.51
1:B:413:ARG:HG2	1:B:414:LYS:N	2.25	0.51
1:B:430:GLU:O	1:B:433:SER:HB3	2.10	0.51
4:A:1520:DGT:O2B	4:A:1520:DGT:H4'	2.11	0.51
1:B:377:TYR:HB2	1:B:399:SER:HB2	1.93	0.51
1:A:73:GLN:O	1:A:73:GLN:HG2	2.10	0.50
1:B:288:THR:HG22	1:B:288:THR:O	2.11	0.50
2:E:13:DC:H5'	2:E:13:DC:H6	1.74	0.50
1:A:215:PRO:C	1:A:217:ASP:N	2.70	0.50
1:A:222:PHE:CD1	1:A:222:PHE:N	2.80	0.50
1:A:330:ASN:C	1:A:330:ASN:ND2	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:O	1:A:425:ILE:HG22	2.11	0.50
1:B:135:MET:HA	1:B:135:MET:CE	2.38	0.50
1:B:388:SER:C	1:B:390:THR:N	2.68	0.50
1:B:418:VAL:O	1:B:510:GLY:HA2	2.11	0.50
1:B:461:LYS:HD2	1:B:467:VAL:HG22	1.93	0.50
2:E:3:DG:N1	3:F:16:DC:N4	2.59	0.50
3:T:17:DC:H2"	3:T:18:DC:H5"	1.94	0.50
1:A:107:ASP:OD1	1:A:108:MET:O	2.29	0.50
1:B:135:MET:HE1	1:B:151:ALA:C	2.36	0.50
1:B:52:ASN:OD1	1:B:465:PHE:HB2	2.11	0.50
1:B:417:SER:HB3	1:B:512:ARG:CG	2.40	0.50
1:B:473:THR:HG21	2:E:6:DA:OP1	2.12	0.50
1:B:63:ARG:NH2	1:B:364:MET:HE1	2.26	0.50
1:B:135:MET:HE2	1:B:136:LEU:N	2.25	0.50
1:B:184:ILE:O	1:B:187:ASP:HB2	2.12	0.50
1:A:473:THR:HG23	2:P:6:DA:OP2	2.12	0.50
1:A:514:SER:O	1:A:515:SER:HB2	2.12	0.50
1:B:207:HIS:NE2	1:B:211:ARG:HD2	2.27	0.50
1:B:299:PHE:O	1:B:302:GLU:HB3	2.11	0.50
1:B:347:LYS:HB3	1:B:347:LYS:HZ2	1.76	0.50
1:A:74:ILE:HG23	1:A:78:GLN:NE2	2.24	0.50
1:A:153:PRO:HB2	1:A:155:PHE:CE2	2.47	0.50
1:B:165:ILE:O	1:B:167:VAL:HG23	2.12	0.50
1:B:389:GLU:O	1:B:393:HIS:HB2	2.12	0.50
2:E:7:DA:H5'	2:E:7:DA:C8	2.46	0.49
1:A:34:GLU:C	1:A:36:ILE:H	2.19	0.49
1:B:323:CYS:O	1:B:324:SER:C	2.53	0.49
1:A:107:ASP:CG	1:A:328:LYS:NZ	2.67	0.49
1:A:409:ARG:O	1:A:411:GLY:N	2.45	0.49
1:B:120:ASN:O	1:B:120:ASN:ND2	2.45	0.49
1:B:213:ASN:C	1:B:215:PRO:CD	2.84	0.49
1:B:462:ASN:HB3	1:B:464:ASN:OD1	2.12	0.49
1:B:209:GLU:O	1:B:212:GLN:HB2	2.11	0.49
1:A:153:PRO:CG	1:A:156:ILE:HD12	2.42	0.49
1:B:108:MET:CA	1:B:309:ALA:HA	2.29	0.49
1:B:134:SER:O	1:B:135:MET:HG2	2.13	0.49
1:B:427:LYS:O	1:B:430:GLU:HB3	2.13	0.49
1:B:461:LYS:CG	1:B:467:VAL:HG22	2.43	0.49
1:A:151:ALA:HB2	4:A:1520:DGT:HN2	1.77	0.49
1:A:456:VAL:O	1:A:471:ALA:HB1	2.13	0.49
1:B:111:PHE:O	1:B:114:ALA:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:ILE:HD11	1:B:345:PHE:CD2	2.47	0.49
1:A:202:LEU:HD12	1:A:202:LEU:N	2.28	0.49
1:A:463:VAL:HG23	1:A:505:ARG:O	2.12	0.49
1:B:161:CYS:O	1:B:164:LEU:HB2	2.13	0.49
1:B:60:VAL:O	1:B:63:ARG:N	2.46	0.49
1:B:497:ASP:O	1:B:498:ALA:C	2.55	0.49
1:A:105:HIS:HE2	1:A:199:GLU:HG2	1.78	0.48
1:B:54:LEU:O	1:B:56:LYS:N	2.46	0.48
1:B:52:ASN:O	1:B:56:LYS:HB2	2.13	0.48
1:B:390:THR:O	1:B:391:SER:C	2.56	0.48
1:B:446:LEU:C	1:B:448:LYS:H	2.19	0.48
1:B:136:LEU:HD11	1:B:157:ALA:CB	2.43	0.48
1:B:480:THR:OG1	1:B:483:GLU:HB2	2.12	0.48
1:A:99:LEU:HD23	1:A:337:PRO:O	2.12	0.48
1:A:138:THR:HG22	1:A:139:SER:N	2.29	0.48
1:A:442:LEU:HD23	1:A:511:VAL:HG12	1.95	0.48
1:B:391:SER:O	1:B:394:TYR:HB3	2.13	0.48
1:A:223:ILE:O	1:A:224:LYS:HB3	2.13	0.48
1:A:506:LEU:HD21	1:A:509:MET:HE3	1.95	0.48
1:B:316:ASN:ND2	1:B:403:GLY:HA3	2.29	0.48
1:B:414:LYS:HB2	3:F:9:DT:OP2	2.14	0.48
1:A:81:LYS:HD3	1:A:81:LYS:C	2.37	0.48
1:B:388:SER:C	1:B:390:THR:H	2.21	0.48
1:B:462:ASN:CB	1:B:464:ASN:OD1	2.61	0.48
1:B:478:VAL:HG12	1:B:479:SER:N	2.27	0.48
1:A:292:GLU:OE1	1:A:295:LYS:HD2	2.13	0.48
1:A:411:GLY:O	1:A:412:GLU:C	2.56	0.48
1:A:455:THR:CB	1:A:473:THR:HG22	2.43	0.48
1:B:365:LEU:HB3	1:B:370:ILE:HB	1.94	0.48
1:A:64:ILE:O	1:A:67:MET:N	2.44	0.48
1:A:74:ILE:CG2	1:A:79:LEU:HD13	2.42	0.48
1:B:109:ASP:OD2	1:B:330:ASN:N	2.47	0.48
1:B:181:VAL:C	1:B:183:GLU:N	2.70	0.48
1:B:411:GLY:O	1:B:412:GLU:C	2.55	0.48
1:B:136:LEU:CD1	1:B:157:ALA:HB2	2.44	0.48
1:B:292:GLU:C	1:B:294:VAL:H	2.21	0.48
1:B:377:TYR:O	1:B:380:ARG:HG2	2.14	0.48
1:A:52:ASN:ND2	1:A:466:GLU:OE2	2.47	0.47
1:B:287:GLY:N	1:B:292:GLU:HG2	2.29	0.47
1:B:327:ASN:HD22	1:B:333:TYR:HB2	1.77	0.47
1:B:444:GLN:O	1:B:448:LYS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:N	1:A:336:LEU:HD23	2.29	0.47
1:B:211:ARG:NH2	1:B:296:GLU:OE2	2.42	0.47
1:B:407:LEU:HD12	1:B:407:LEU:N	2.20	0.47
2:E:4:DG:C1'	2:E:5:DG:H5''	2.41	0.47
1:A:127:PRO:HA	1:A:140:ASN:HD21	1.79	0.47
1:B:210:GLU:C	1:B:212:GLN:N	2.72	0.47
1:B:292:GLU:C	1:B:294:VAL:N	2.71	0.47
1:A:74:ILE:HG21	1:A:79:LEU:HD13	1.95	0.47
1:B:47:SER:O	1:B:49:PHE:N	2.47	0.47
1:B:391:SER:OG	3:F:12:DT:OP1	2.32	0.47
1:A:102:THR:H	1:A:205:THR:HB	1.79	0.47
1:A:398:ILE:HD12	1:A:398:ILE:N	2.30	0.47
1:B:216:GLU:OE2	1:B:216:GLU:HA	2.15	0.47
1:A:203:ASN:C	1:A:205:THR:N	2.69	0.47
1:A:394:TYR:CE1	1:A:398:ILE:HD11	2.49	0.47
1:B:128:ILE:CG1	1:B:140:ASN:HB2	2.45	0.47
1:B:185:LEU:O	1:B:187:ASP:N	2.47	0.47
1:B:215:PRO:HA	1:B:219:ARG:HH21	1.79	0.47
1:B:312:GLY:HA3	1:B:323:CYS:HB2	1.96	0.47
1:B:485:PHE:O	1:B:489:LYS:CB	2.63	0.47
1:A:382:LEU:CD2	1:A:386:LEU:HG	2.44	0.47
1:B:75:THR:N	1:B:78:GLN:OE1	2.48	0.47
1:B:170:ASN:O	1:B:173:LYS:N	2.48	0.47
2:P:10:DA:H1'	2:P:11:DT:H5'	1.96	0.47
3:T:9:DT:H2''	3:T:10:DC:C6	2.50	0.47
1:B:71:LYS:C	1:B:73:GLN:N	2.73	0.47
1:A:178:SER:OG	1:A:182:LYS:HE3	2.15	0.46
1:B:133:MET:O	1:B:154:GLY:HA3	2.14	0.46
1:B:305:THR:C	1:B:307:LEU:H	2.23	0.46
3:T:7:DA:H2''	3:T:8:DA:C5'	2.45	0.46
1:B:192:PHE:CD1	1:B:192:PHE:C	2.93	0.46
1:B:358:GLY:O	1:B:359:LYS:C	2.58	0.46
3:T:3:DA:H4'	3:T:3:DA:OP1	2.16	0.46
1:A:436:GLN:HA	1:A:485:PHE:CE2	2.50	0.46
1:B:431:GLN:HE22	1:B:506:LEU:HD13	1.73	0.46
1:A:208:LEU:HD11	1:A:290:ALA:CB	2.38	0.46
1:A:282:ASN:O	1:A:283:SER:C	2.58	0.46
1:B:158:LYS:C	1:B:160:LEU:N	2.71	0.46
1:A:120:ASN:ND2	1:A:122:GLU:HB3	2.30	0.46
1:A:220:ARG:CB	1:A:285:VAL:HG22	2.46	0.46
1:A:463:VAL:O	1:A:463:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:PHE:CD2	1:A:500:PHE:C	2.92	0.46
1:A:375:GLU:H	1:A:375:GLU:HG2	1.57	0.46
1:B:149:ARG:CG	1:B:152:MET:HE3	2.45	0.46
1:B:349:LEU:HD23	1:B:350:PRO:N	2.31	0.46
1:B:407:LEU:H	1:B:407:LEU:CD1	2.12	0.46
1:B:449:GLU:HB2	1:B:451:LEU:CD2	2.44	0.46
2:P:8:DG:H1'	2:P:9:DG:H5''	1.98	0.46
3:T:11:DC:H2''	3:T:12:DT:C7	2.46	0.46
1:A:170:ASN:O	1:A:173:LYS:HB3	2.16	0.46
1:B:311:ALA:O	1:B:332:GLN:HA	2.15	0.46
1:A:497:ASP:O	1:A:498:ALA:C	2.58	0.46
1:B:67:MET:O	1:B:70:GLN:HB2	2.16	0.46
1:B:305:THR:HG23	1:B:307:LEU:H	1.79	0.46
1:B:349:LEU:C	1:B:349:LEU:CD2	2.89	0.46
1:B:135:MET:HE2	1:B:135:MET:CA	2.44	0.45
1:B:298:ARG:NH2	1:B:330:ASN:OD1	2.49	0.45
1:B:435:CYS:O	1:B:438:LEU:HB2	2.16	0.45
1:A:170:ASN:OD1	1:A:170:ASN:C	2.59	0.45
1:A:339:ARG:O	1:A:343:MET:HG2	2.16	0.45
1:A:342:VAL:O	1:A:346:ILE:HG13	2.16	0.45
2:E:4:DG:C2'	2:E:5:DG:H5''	2.47	0.45
1:A:153:PRO:HG2	1:A:156:ILE:HB	1.98	0.45
1:A:449:GLU:O	1:A:450:ARG:C	2.59	0.45
1:B:34:GLU:C	1:B:36:ILE:N	2.73	0.45
1:B:371:ILE:HG22	1:B:372:THR:CG2	2.47	0.45
1:A:69:GLN:C	1:A:71:LYS:N	2.72	0.45
1:A:128:ILE:HG22	1:A:165:ILE:HB	1.98	0.45
1:B:205:THR:HG23	1:B:206:LYS:N	2.31	0.45
1:B:371:ILE:N	1:B:375:GLU:OE2	2.48	0.45
1:B:128:ILE:HG13	1:B:129:ALA:H	1.80	0.45
1:B:176:ALA:O	1:B:180:GLU:HB2	2.15	0.45
1:B:185:LEU:C	1:B:187:ASP:N	2.74	0.45
2:E:12:DT:H6	2:E:12:DT:H2'	1.59	0.45
1:A:292:GLU:O	1:A:295:LYS:N	2.49	0.45
1:A:372:THR:OG1	1:A:375:GLU:HG2	2.17	0.45
1:A:420:ARG:O	1:A:508:LEU:HD23	2.17	0.45
1:B:45:LYS:CG	1:B:46:GLY:N	2.73	0.45
1:B:434:LEU:O	1:B:438:LEU:HG	2.16	0.45
1:B:438:LEU:O	1:B:439:CYS:C	2.59	0.45
1:A:346:ILE:CD1	1:A:401:GLY:HA3	2.45	0.45
1:A:351:ILE:HG23	1:A:352:ARG:N	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:THR:HG23	1:B:307:LEU:N	2.31	0.45
1:B:366:LYS:C	1:B:368:LEU:H	2.25	0.45
1:B:436:GLN:HB2	1:B:485:PHE:CE1	2.52	0.45
1:B:444:GLN:O	1:B:448:LYS:HE3	2.17	0.45
1:A:74:ILE:HG21	1:A:79:LEU:CD1	2.46	0.45
1:A:97:ARG:HG2	1:A:99:LEU:HD11	1.96	0.45
1:A:195:MET:HB2	1:A:199:GLU:HB3	1.98	0.45
1:A:462:ASN:ND2	1:A:464:ASN:H	2.15	0.45
1:A:482:GLU:N	1:A:482:GLU:OE1	2.50	0.45
1:B:50:TYR:O	1:B:53:GLU:N	2.50	0.45
1:B:120:ASN:N	1:B:121:PRO:HD3	2.30	0.45
1:A:63:ARG:NH2	1:A:364:MET:HE1	2.32	0.45
1:B:114:ALA:HA	1:B:117:MET:HE2	1.98	0.45
1:A:471:ALA:HA	1:A:491:LEU:HD13	1.99	0.44
1:B:178:SER:O	1:B:181:VAL:HG12	2.16	0.44
1:B:412:GLU:HG3	1:B:413:ARG:N	2.32	0.44
2:E:10:DA:H2''	2:E:11:DT:H5'	1.99	0.44
1:A:447:GLN:O	1:A:448:LYS:C	2.61	0.44
1:B:316:ASN:ND2	1:B:318:MET:HB3	2.32	0.44
1:B:359:LYS:HE3	1:B:360:VAL:HG23	1.99	0.44
1:B:382:LEU:HD22	1:B:386:LEU:HG	1.98	0.44
1:B:465:PHE:N	1:B:465:PHE:CD1	2.85	0.44
3:T:18:DC:H6	3:T:18:DC:H5'	1.83	0.44
1:A:326:LYS:HG2	1:A:333:TYR:CD1	2.51	0.44
4:B:1520:DGT:PB	4:B:1520:DGT:C5'	3.02	0.44
1:A:93:LEU:HD13	1:A:397:HIS:CE1	2.52	0.44
1:A:128:ILE:N	1:A:140:ASN:HD21	2.10	0.44
1:B:104:VAL:O	1:B:201:TYR:HA	2.17	0.44
1:A:71:LYS:HE3	1:A:382:LEU:HD11	1.99	0.44
1:A:389:GLU:HA	1:A:392:TRP:NE1	2.32	0.44
1:B:105:HIS:O	1:B:311:ALA:HA	2.18	0.44
1:B:208:LEU:HD23	1:B:208:LEU:HA	1.73	0.44
1:B:40:ILE:C	1:B:42:GLU:N	2.76	0.44
1:B:95:GLN:C	1:B:97:ARG:H	2.25	0.44
1:B:513:ILE:O	1:B:513:ILE:HG23	2.18	0.44
1:A:323:CYS:C	1:A:325:ASP:N	2.74	0.44
1:A:201:TYR:CZ	1:A:317:THR:HG23	2.52	0.44
1:A:128:ILE:HD12	1:A:128:ILE:C	2.43	0.44
1:A:302:GLU:HA	1:A:307:LEU:O	2.18	0.44
1:A:346:ILE:HD11	1:A:401:GLY:CA	2.46	0.44
1:A:365:LEU:HD21	1:A:395:PHE:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:PHE:C	1:A:422:PHE:CD1	2.96	0.44
1:A:41:MET:HE1	1:A:50:TYR:CE2	2.52	0.43
1:A:483:GLU:H	1:A:483:GLU:HG3	1.54	0.43
1:B:328:LYS:HE2	1:B:328:LYS:CA	2.46	0.43
2:P:5:DG:H5'	2:P:5:DG:H8	1.83	0.43
1:A:37:ASN:C	1:A:39:ILE:H	2.25	0.43
1:A:41:MET:HE3	1:A:41:MET:HA	1.99	0.43
1:A:115:VAL:HG22	1:A:307:LEU:HD11	2.00	0.43
1:A:352:ARG:HD3	1:A:358:GLY:O	2.18	0.43
1:B:420:ARG:C	1:B:508:LEU:HD22	2.43	0.43
1:B:455:THR:HB	1:B:514:SER:O	2.18	0.43
1:A:120:ASN:C	1:A:120:ASN:HD22	2.26	0.43
1:A:289:SER:O	1:A:292:GLU:HB2	2.18	0.43
1:B:55:LYS:HD2	1:B:55:LYS:HA	1.82	0.43
1:B:219:ARG:HH11	1:B:219:ARG:CB	2.31	0.43
1:B:163:GLN:O	1:B:165:ILE:HG13	2.18	0.43
1:A:84:LEU:O	1:A:85:GLN:C	2.62	0.43
1:A:128:ILE:N	1:A:140:ASN:ND2	2.42	0.43
1:A:189:ASP:OD2	1:A:189:ASP:C	2.61	0.43
1:A:427:LYS:HB3	1:A:430:GLU:CD	2.44	0.43
1:A:459:LYS:HG3	1:A:469:THR:HG22	2.00	0.43
1:A:133:MET:HE1	1:A:158:LYS:NZ	2.32	0.43
1:A:178:SER:O	1:A:181:VAL:HG12	2.18	0.43
1:A:203:ASN:ND2	1:A:205:THR:HB	2.34	0.43
1:B:49:PHE:CD2	3:F:4:DC:C4	3.06	0.43
1:B:495:GLU:O	1:B:496:ILE:C	2.61	0.43
1:B:500:PHE:C	1:B:502:HIS:N	2.76	0.43
4:B:1520:DGT:H5'A	4:B:1520:DGT:O1B	2.18	0.43
1:A:80:ARG:NH2	1:B:95:GLN:O	2.42	0.43
1:A:517:PRO:O	1:A:518:ASN:HB2	2.18	0.43
1:B:400:LEU:HD23	1:B:400:LEU:HA	1.82	0.43
1:B:508:LEU:C	1:B:508:LEU:CD1	2.92	0.43
1:A:56:LYS:NZ	1:A:56:LYS:HB3	2.33	0.43
1:A:123:LEU:HD13	1:A:128:ILE:HG21	2.00	0.43
1:A:163:GLN:NE2	6:A:2006:HOH:O	2.43	0.43
1:A:366:LYS:HE2	1:A:371:ILE:CD1	2.49	0.43
1:B:203:ASN:C	1:B:205:THR:N	2.74	0.43
1:B:205:THR:CG2	1:B:206:LYS:N	2.82	0.43
1:B:219:ARG:HB3	1:B:219:ARG:NH1	2.32	0.43
1:B:294:VAL:HG12	1:B:294:VAL:O	2.18	0.43
1:B:223:ILE:HD12	1:B:282:ASN:CA	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:DG:H2''	2:E:5:DG:H5''	2.00	0.43
1:A:209:GLU:O	1:A:212:GLN:HG2	2.19	0.43
1:B:45:LYS:CG	1:B:46:GLY:H	2.29	0.43
1:B:214:TRP:O	1:B:215:PRO:C	2.61	0.43
1:B:370:ILE:HG12	1:B:379:GLN:HG3	2.00	0.43
1:B:490:GLU:O	1:B:493:LYS:HB3	2.18	0.43
1:A:120:ASN:ND2	1:A:120:ASN:C	2.77	0.42
1:A:461:LYS:HG3	1:A:467:VAL:CG2	2.48	0.42
1:B:217:ASP:CG	1:B:218:LYS:N	2.77	0.42
1:B:288:THR:O	1:B:288:THR:CG2	2.67	0.42
1:B:93:LEU:HD13	1:B:397:HIS:CD2	2.54	0.42
1:B:336:LEU:HA	1:B:337:PRO:HD3	1.78	0.42
2:E:3:DG:H2''	2:E:4:DG:C8	2.54	0.42
1:A:184:ILE:HD12	1:A:301:ILE:HA	2.01	0.42
1:A:208:LEU:CD1	1:A:290:ALA:HB2	2.41	0.42
1:A:151:ALA:HB2	4:A:1520:DGT:N2	2.34	0.42
1:A:490:GLU:OE2	1:A:490:GLU:HA	2.20	0.42
1:B:366:LYS:C	1:B:368:LEU:N	2.77	0.42
1:A:340:GLN:NE2	1:A:340:GLN:CA	2.76	0.42
1:A:452:LYS:CG	1:A:479:SER:OG	2.67	0.42
1:A:493:LYS:HE3	1:A:497:ASP:OD1	2.19	0.42
1:B:181:VAL:CG2	1:B:301:ILE:HG12	2.49	0.42
1:A:99:LEU:CD1	1:A:99:LEU:N	2.82	0.42
1:B:174:TYR:O	1:B:177:VAL:N	2.51	0.42
1:B:309:ALA:O	1:B:330:ASN:HA	2.19	0.42
1:B:316:ASN:HD22	1:B:318:MET:N	2.16	0.42
1:B:328:LYS:HB3	1:B:329:PRO:CD	2.41	0.42
1:A:49:PHE:HB2	1:A:465:PHE:CZ	2.55	0.42
1:A:181:VAL:HG23	1:A:301:ILE:HG12	2.01	0.42
1:B:140:ASN:HB3	1:B:143:ALA:HB2	2.02	0.42
1:B:290:ALA:O	1:B:291:GLN:C	2.62	0.42
1:B:446:LEU:C	1:B:448:LYS:N	2.77	0.42
3:F:2:DC:O2	3:F:2:DC:C2'	2.60	0.42
1:A:35:LYS:NZ	1:A:38:LYS:HD3	2.33	0.42
1:A:44:THR:O	1:A:45:LYS:C	2.62	0.42
1:B:294:VAL:O	1:B:294:VAL:CG1	2.66	0.42
1:A:189:ASP:OD2	1:A:191:ASN:O	2.37	0.42
1:B:213:ASN:CA	1:B:215:PRO:HD3	2.49	0.42
1:B:478:VAL:CG1	1:B:479:SER:N	2.83	0.42
1:A:37:ASN:HD22	1:A:37:ASN:H	1.68	0.41
1:B:118:ARG:NE	1:B:307:LEU:HD23	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:SER:O	1:B:418:VAL:HG13	2.19	0.41
1:B:491:LEU:HD23	1:B:491:LEU:HA	1.86	0.41
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.86	0.41
1:A:485:PHE:CD1	1:A:485:PHE:C	2.98	0.41
1:B:283:SER:O	1:B:284:VAL:HG13	2.20	0.41
1:A:377:TYR:O	1:A:380:ARG:HB3	2.20	0.41
1:A:380:ARG:HG2	1:A:380:ARG:HH11	1.85	0.41
1:A:442:LEU:HD22	1:A:511:VAL:O	2.19	0.41
1:A:486:ALA:O	1:A:489:LYS:HG2	2.20	0.41
1:B:212:GLN:OE1	1:B:288:THR:HG21	2.19	0.41
1:A:128:ILE:HG13	1:A:140:ASN:ND2	2.27	0.41
1:A:350:PRO:HB2	1:A:353:LYS:HG2	2.02	0.41
1:B:138:THR:CG2	1:B:139:SER:N	2.84	0.41
1:B:296:GLU:O	1:B:300:ARG:HG3	2.20	0.41
3:T:5:8OG:H2''	3:T:5:8OG:O5'	2.21	0.41
3:T:16:DC:H2''	3:T:17:DC:C6	2.55	0.41
1:A:109:ASP:C	1:A:111:PHE:N	2.78	0.41
1:A:203:ASN:O	1:A:205:THR:N	2.53	0.41
1:A:349:LEU:HD12	1:A:350:PRO:HD2	2.01	0.41
1:B:208:LEU:HD11	1:B:290:ALA:CA	2.50	0.41
1:B:346:ILE:HA	1:B:346:ILE:HD12	1.77	0.41
1:A:79:LEU:HD12	1:A:79:LEU:HA	1.83	0.41
1:A:85:GLN:O	1:A:88:ARG:HB3	2.21	0.41
1:A:108:MET:SD	1:A:309:ALA:HB2	2.61	0.41
1:A:459:LYS:HA	1:A:469:THR:HG22	2.03	0.41
1:B:74:ILE:HA	1:B:78:GLN:OE1	2.20	0.41
1:B:371:ILE:HB	1:B:375:GLU:OE2	2.21	0.41
4:B:1520:DGT:O1B	4:B:1520:DGT:O1A	2.37	0.41
1:A:485:PHE:O	1:A:489:LYS:HG2	2.20	0.41
1:B:483:GLU:O	1:B:486:ALA:HB3	2.20	0.41
1:B:500:PHE:C	1:B:502:HIS:H	2.27	0.41
1:A:207:HIS:CD2	1:A:207:HIS:C	2.98	0.41
1:A:455:THR:OG1	1:A:473:THR:CG2	2.58	0.41
1:B:115:VAL:HG22	1:B:307:LEU:CD1	2.47	0.41
1:B:121:PRO:O	1:B:122:GLU:CB	2.55	0.41
1:B:317:THR:OG1	1:B:318:MET:N	2.53	0.41
1:A:197:LEU:HA	1:A:197:LEU:HD23	1.76	0.41
1:B:71:LYS:O	1:B:74:ILE:HG13	2.20	0.41
1:B:108:MET:HE3	1:B:108:MET:HB2	1.68	0.41
1:B:165:ILE:O	1:B:167:VAL:N	2.53	0.41
1:B:218:LYS:HD2	1:B:218:LYS:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:HD23	1:B:350:PRO:O	2.21	0.41
1:B:423:SER:O	1:B:424:GLU:C	2.63	0.41
1:B:516:PHE:N	1:B:517:PRO:CD	2.81	0.41
1:A:110:ALA:N	4:A:1520:DGT:O1G	2.49	0.41
1:A:192:PHE:CD1	1:A:192:PHE:C	2.99	0.41
1:A:411:GLY:O	1:A:412:GLU:O	2.38	0.41
1:B:354:VAL:HG23	1:B:355:SER:O	2.20	0.41
1:B:449:GLU:O	1:B:451:LEU:HD22	2.21	0.41
1:A:69:GLN:C	1:A:71:LYS:H	2.29	0.40
1:A:199:GLU:O	1:A:200:ALA:CB	2.69	0.40
1:A:389:GLU:C	1:A:391:SER:N	2.79	0.40
1:B:49:PHE:CE2	3:F:4:DC:N3	2.89	0.40
1:B:75:THR:OG1	1:B:78:GLN:HG3	2.22	0.40
1:B:219:ARG:CB	1:B:219:ARG:NH1	2.83	0.40
1:B:388:SER:O	1:B:390:THR:N	2.54	0.40
2:E:4:DG:H2'	2:E:5:DG:H5'	2.03	0.40
1:A:443:ALA:HB2	1:A:484:ILE:HD12	2.03	0.40
1:B:456:VAL:HG22	1:B:513:ILE:HD13	2.03	0.40
1:A:149:ARG:HG2	1:A:152:MET:CE	2.46	0.40
1:A:445:ASP:O	1:A:448:LYS:HE2	2.20	0.40
1:B:316:ASN:HD21	1:B:318:MET:HB3	1.86	0.40
3:T:3:DA:OP1	3:T:3:DA:C4'	2.69	0.40
3:T:12:DT:C2'	3:T:13:DT:H5'	2.34	0.40
4:A:1520:DGT:O4'	2:P:13:DC:H2'	2.21	0.40
1:B:42:GLU:CD	1:B:42:GLU:C	2.89	0.40
1:B:446:LEU:HD13	1:B:513:ILE:HG21	2.02	0.40
1:B:482:GLU:CD	1:B:482:GLU:N	2.78	0.40
1:B:513:ILE:HD12	1:B:513:ILE:HA	1.94	0.40
1:A:107:ASP:OD2	4:A:1520:DGT:O1B	2.40	0.40
1:A:323:CYS:O	1:A:324:SER:C	2.65	0.40
1:A:422:PHE:C	1:A:422:PHE:HD1	2.29	0.40
1:A:463:VAL:CG2	1:A:505:ARG:HB3	2.51	0.40
1:A:499:ASP:OD1	1:A:499:ASP:N	2.54	0.40
1:A:514:SER:O	1:A:515:SER:CB	2.69	0.40
1:B:119:ASP:O	1:B:120:ASN:CB	2.70	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	428/508 (84%)	337 (79%)	69 (16%)	22 (5%)	1	10
1	B	426/508 (84%)	307 (72%)	79 (18%)	40 (9%)	0	2
All	All	854/1016 (84%)	644 (75%)	148 (17%)	62 (7%)	1	5

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	47	SER
1	A	72	ALA
1	A	73	GLN
1	A	124	LYS
1	A	283	SER
1	A	410	ASP
1	A	411	GLY
1	A	412	GLU
1	A	428	ALA
1	A	450	ARG
1	A	517	PRO
1	B	120	ASN
1	B	121	PRO
1	B	129	ALA
1	B	169	PRO
1	B	170	ASN
1	B	204	ILE
1	B	217	ASP
1	B	462	ASN
1	B	498	ALA
1	B	516	PHE
1	A	45	LYS
1	A	111	PHE
1	A	200	ALA
1	A	389	GLU

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Mol	Chain	Res	Type
1	A	515	SER
1	B	72	ALA
1	B	109	ASP
1	B	110	ALA
1	B	128	ILE
1	B	166	ILE
1	B	171	PHE
1	B	186	ALA
1	B	283	SER
1	B	347	LYS
1	B	411	GLY
1	B	427	LYS
1	B	497	ASP
1	B	503	PRO
1	B	505	ARG
1	A	193	MET
1	A	330	ASN
1	A	482	GLU
1	B	55	LYS
1	B	111	PHE
1	B	216	GLU
1	B	479	SER
1	A	135	MET
1	B	45	LYS
1	B	126	LYS
1	B	215	PRO
1	B	515	SER
1	A	447	GLN
1	B	160	LEU
1	B	304	LYS
1	B	447	GLN
1	A	204	ILE
1	B	359	LYS
1	B	412	GLU
1	B	337	PRO
1	B	214	TRP
1	B	425	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	384/454 (85%)	350 (91%)	34 (9%)	9	30
1	B	382/454 (84%)	352 (92%)	30 (8%)	11	36
All	All	766/908 (84%)	702 (92%)	64 (8%)	10	33

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	57	GLU
1	A	60	VAL
1	A	79	LEU
1	A	80	ARG
1	A	81	LYS
1	A	93	LEU
1	A	99	LEU
1	A	101	ASN
1	A	118	ARG
1	A	144	ARG
1	A	163	GLN
1	A	191	ASN
1	A	222	PHE
1	A	288	THR
1	A	293	VAL
1	A	302	GLU
1	A	325	ASP
1	A	336	LEU
1	A	368	LEU
1	A	375	GLU
1	A	379	GLN
1	A	382	LEU
1	A	391	SER
1	A	405	THR
1	A	407	LEU
1	A	422	PHE
1	A	444	GLN
1	A	483	GLU
1	A	487	ILE
1	A	499	ASP

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Mol	Chain	Res	Type
1	A	508	LEU
1	A	512	ARG
1	A	516	PHE
1	B	60	VAL
1	B	77	GLN
1	B	92	GLU
1	B	101	ASN
1	B	120	ASN
1	B	121	PRO
1	B	125	ASP
1	B	135	MET
1	B	155	PHE
1	B	293	VAL
1	B	328	LYS
1	B	346	ILE
1	B	347	LYS
1	B	354	VAL
1	B	363	LYS
1	B	379	GLN
1	B	382	LEU
1	B	393	HIS
1	B	407	LEU
1	B	420	ARG
1	B	430	GLU
1	B	458	ILE
1	B	466	GLU
1	B	469	THR
1	B	473	THR
1	B	480	THR
1	B	504	LEU
1	B	508	LEU
1	B	516	PHE
1	B	519	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	52	ASN
1	A	66	ASN
1	A	70	GLN
1	A	73	GLN

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Mol	Chain	Res	Type
1	A	77	GLN
1	A	78	GLN
1	A	83	GLN
1	A	120	ASN
1	A	140	ASN
1	A	203	ASN
1	A	213	ASN
1	A	282	ASN
1	A	303	GLN
1	A	330	ASN
1	A	334	GLN
1	A	340	GLN
1	A	379	GLN
1	A	444	GLN
1	A	462	ASN
1	A	518	ASN
1	B	73	GLN
1	B	77	GLN
1	B	83	GLN
1	B	95	GLN
1	B	101	ASN
1	B	120	ASN
1	B	140	ASN
1	B	203	ASN
1	B	213	ASN
1	B	282	ASN
1	B	316	ASN
1	B	327	ASN
1	B	330	ASN
1	B	334	GLN
1	B	379	GLN
1	B	397	HIS
1	B	431	GLN
1	B	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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$
3	8OG	F	5	3	22,25,26	1.50	4 (18%)	26,37,40	2.16	9 (34%)
3	8OG	T	5	3	22,25,26	1.49	4 (18%)	26,37,40	2.14	8 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8OG	F	5	3	-	0/7/21/22	0/3/3/3
3	8OG	T	5	3	-	0/7/21/22	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	5	8OG	C8-N9	-4.15	1.33	1.40
3	T	5	8OG	C8-N9	-4.13	1.33	1.40
3	F	5	8OG	C4-N9	-3.10	1.33	1.39
3	T	5	8OG	C4-N9	-2.99	1.33	1.39
3	F	5	8OG	C8-N7	-2.73	1.33	1.38
3	T	5	8OG	C8-N7	-2.70	1.33	1.38
3	F	5	8OG	C5-N7	-2.64	1.33	1.37
3	T	5	8OG	C5-N7	-2.62	1.33	1.37

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	T	5	8OG	C2-N3-C4	5.71	122.14	112.30
3	F	5	8OG	C2-N3-C4	5.52	121.80	112.30
3	T	5	8OG	N9-C4-N3	4.68	131.97	126.13
3	F	5	8OG	N9-C4-N3	4.51	131.77	126.13
3	T	5	8OG	N7-C8-N9	4.11	111.19	106.61
3	F	5	8OG	N7-C8-N9	4.09	111.17	106.61
3	T	5	8OG	C2-N1-C6	-3.15	119.41	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	5	8OG	C2-N1-C6	-3.13	119.43	125.11
3	F	5	8OG	O6-C6-C5	-2.83	120.43	127.26
3	T	5	8OG	O6-C6-C5	-2.73	120.67	127.26
3	T	5	8OG	C5-C6-N1	2.59	119.25	112.13
3	F	5	8OG	C5-C6-N1	2.58	119.20	112.13
3	F	5	8OG	O4'-C1'-C2'	-2.17	102.19	106.25
3	F	5	8OG	C3'-C2'-C1'	-2.12	97.42	102.60
3	F	5	8OG	C5-N7-C8	-2.10	106.57	109.47
3	T	5	8OG	N1-C2-N3	-2.06	119.55	123.32
3	T	5	8OG	C3'-C2'-C1'	-2.02	97.66	102.60

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	8OG	1	0
3	T	5	8OG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
4	DGT	A	1520	5	32,33,33	1.12	1 (3%)	48,52,52	2.13	19 (39%)
4	DGT	B	1520	5	32,33,33	1.15	1 (3%)	48,52,52	2.23	20 (41%)

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	DGT	A	1520	5	-	4/22/34/34	0/3/3/3
4	DGT	B	1520	5	-	6/22/34/34	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1520	DGT	C5-N7	-2.85	1.33	1.39
4	B	1520	DGT	C5-N7	-2.83	1.33	1.39

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1520	DGT	C2-N3-C4	5.47	121.72	112.30
4	A	1520	DGT	C2-N3-C4	5.37	121.56	112.30
4	B	1520	DGT	C5-C4-N3	-4.82	120.71	128.39
4	A	1520	DGT	C5-C4-N3	-4.66	120.97	128.39
4	B	1520	DGT	C4'-O4'-C1'	-4.47	98.88	109.51
4	A	1520	DGT	O3A-PA-O2A	4.08	122.97	110.70
4	B	1520	DGT	O1G-PG-O3B	-3.86	91.68	104.64
4	A	1520	DGT	O1G-PG-O3B	-3.84	91.75	104.64
4	B	1520	DGT	O3A-PA-O2A	3.71	121.86	110.70
4	A	1520	DGT	O2G-PG-O3B	-3.70	92.21	104.64
4	B	1520	DGT	O2G-PG-O3B	-3.31	93.54	104.64
4	B	1520	DGT	N9-C4-N3	3.28	132.51	125.95
4	B	1520	DGT	O4'-C1'-N9	3.18	113.50	107.86
4	A	1520	DGT	N9-C4-N3	3.10	132.16	125.95
4	B	1520	DGT	C2-N1-C6	-3.09	119.50	125.11
4	A	1520	DGT	C2-N1-C6	-3.06	119.56	125.11
4	B	1520	DGT	O1G-PG-O3G	2.91	122.16	110.83
4	A	1520	DGT	O2G-PG-O3G	2.89	122.10	110.83
4	B	1520	DGT	O2G-PG-O3G	2.88	122.07	110.83
4	A	1520	DGT	C4'-O4'-C1'	-2.82	102.80	109.51
4	A	1520	DGT	O1G-PG-O3G	2.81	121.79	110.83
4	B	1520	DGT	O1A-PA-O5'	-2.79	94.91	107.57
4	B	1520	DGT	O4'-C1'-C2'	-2.50	101.58	106.25
4	A	1520	DGT	O5'-PA-O2A	-2.48	99.13	108.94
4	B	1520	DGT	O5'-PA-O2A	-2.41	99.38	108.94
4	A	1520	DGT	O1A-PA-O5'	-2.31	97.09	107.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1520	DGT	O3B-PG-O3G	-2.30	98.95	111.04
4	A	1520	DGT	N9-C8-N7	-2.19	109.34	113.40
4	B	1520	DGT	O6-C6-C5	-2.18	120.77	126.53
4	A	1520	DGT	O6-C6-C5	-2.18	120.77	126.53
4	A	1520	DGT	C5-C6-N1	2.18	118.79	113.25
4	B	1520	DGT	O3B-PG-O3G	-2.16	99.66	111.04
4	B	1520	DGT	C5-C6-N1	2.13	118.69	113.25
4	A	1520	DGT	C8-N7-C5	2.13	108.06	104.26
4	A	1520	DGT	C4-C5-N7	-2.10	107.34	110.67
4	A	1520	DGT	O1A-PA-O2A	2.08	122.14	112.44
4	B	1520	DGT	O4'-C4'-C5'	2.08	115.99	109.33
4	B	1520	DGT	N9-C8-N7	-2.04	109.61	113.40
4	B	1520	DGT	O1A-PA-O2A	2.03	121.90	112.44

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1520	DGT	C5'-O5'-PA-O3A
4	A	1520	DGT	C5'-O5'-PA-O1A
4	A	1520	DGT	C5'-O5'-PA-O2A
4	B	1520	DGT	PA-O3A-PB-O1B
4	B	1520	DGT	C5'-O5'-PA-O3A
4	B	1520	DGT	PB-O3A-PA-O1A
4	B	1520	DGT	O4'-C4'-C5'-O5'
4	B	1520	DGT	C4'-C5'-O5'-PA
4	B	1520	DGT	PA-O3A-PB-O2B
4	A	1520	DGT	O4'-C4'-C5'-O5'

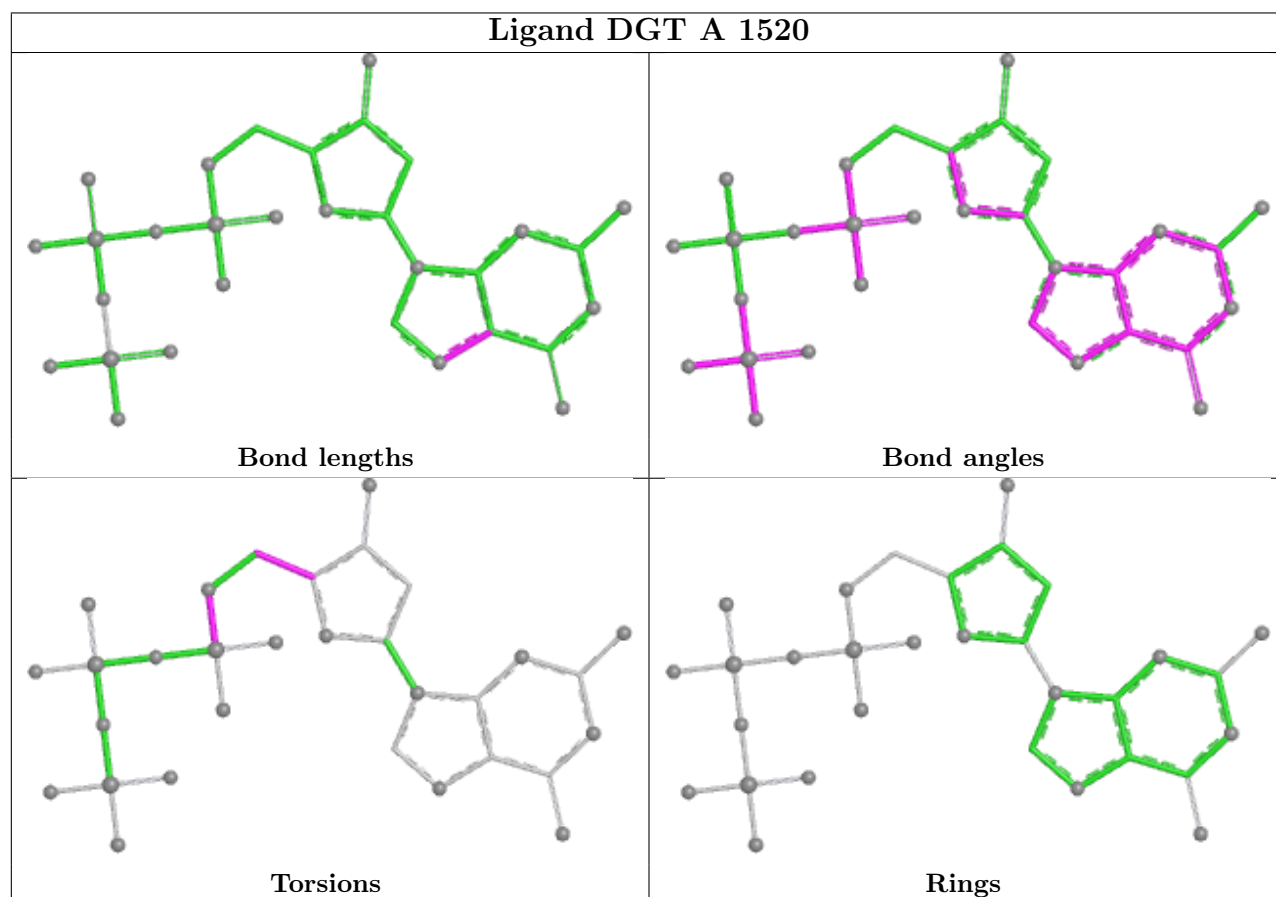
There are no ring outliers.

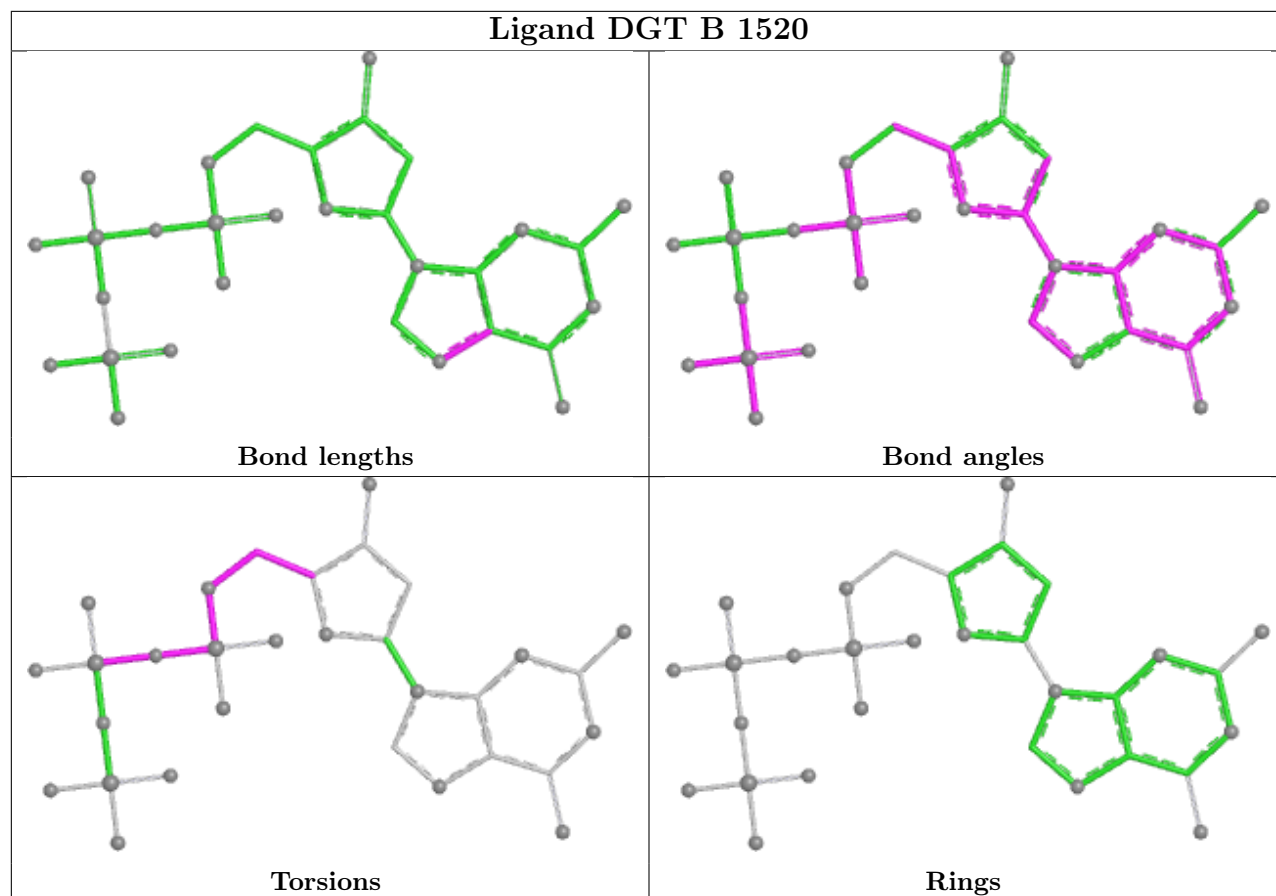
2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1520	DGT	6	0
4	B	1520	DGT	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	432/508 (85%)	0.34	29 (6%)	24 13	49, 79, 114, 129	35 (8%)
1	B	430/508 (84%)	0.63	50 (11%)	9 6	55, 102, 134, 153	54 (12%)
2	E	11/13 (84%)	1.29	2 (18%)	3 2	90, 101, 136, 145	4 (36%)
2	P	13/13 (100%)	0.77	2 (15%)	5 3	51, 85, 148, 160	0
3	F	14/18 (77%)	1.42	4 (28%)	1 1	84, 103, 128, 129	6 (42%)
3	T	16/18 (88%)	0.91	2 (12%)	8 5	63, 93, 141, 145	2 (12%)
All	All	916/1078 (84%)	0.52	89 (9%)	13 8	49, 89, 130, 160	101 (11%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	500	PHE	6.0
1	B	459	LYS	5.9
1	B	222	PHE	5.3
1	A	448	LYS	5.3
1	B	199	GLU	5.0
1	B	195	MET	5.0
3	F	2	DC	4.9
3	F	3	DA	4.7
1	B	419	GLU	4.5
1	B	194	ALA	4.3
1	B	420	ARG	4.3
2	E	3	DG	4.3
1	A	465	PHE	4.1
1	B	200	ALA	3.8
1	B	427	LYS	3.6
1	A	516	PHE	3.6
1	B	171	PHE	3.6
1	B	77	GLN	3.6
1	A	468	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	445	ASP	3.5
1	B	179	LYS	3.3
1	B	206	LYS	3.3
1	B	332	GLN	3.3
1	B	489	LYS	3.1
1	A	441	GLU	3.1
1	B	141	TYR	3.1
3	T	3	DA	3.1
1	B	151	ALA	3.1
3	T	2	DC	3.0
1	B	447	GLN	2.9
1	B	450	ARG	2.9
1	A	449	GLU	2.9
1	A	512	ARG	2.9
1	B	429	GLU	2.9
1	A	149	ARG	2.9
1	A	409	ARG	2.9
1	B	152	MET	2.9
3	F	15	DC	2.9
1	B	220	ARG	2.8
1	A	209	GLU	2.8
1	B	116	GLU	2.8
1	A	214	TRP	2.7
1	B	106	ILE	2.7
1	B	306	THR	2.7
1	A	437	GLU	2.6
1	B	470	ARG	2.6
1	A	451	LEU	2.6
1	B	409	ARG	2.6
1	B	454	ARG	2.6
1	A	223	ILE	2.6
1	A	38	LYS	2.6
1	B	299	PHE	2.6
1	B	441	GLU	2.6
1	A	124	LYS	2.6
3	F	14	DC	2.5
1	B	283	SER	2.4
1	A	210	GLU	2.4
1	B	34	GLU	2.4
1	A	184	ILE	2.4
1	B	348	ASP	2.4
1	B	410	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	156	ILE	2.4
1	A	454	ARG	2.4
1	A	467	VAL	2.4
1	B	201	TYR	2.3
1	A	45	LYS	2.3
1	B	510	GLY	2.3
1	B	105	HIS	2.3
1	B	193	MET	2.3
1	B	142	HIS	2.3
1	A	281	GLN	2.3
1	B	431	GLN	2.3
2	E	5	DG	2.2
1	A	218	LYS	2.2
1	B	218	LYS	2.2
1	B	303	GLN	2.2
1	B	315	PRO	2.2
1	A	35	LYS	2.2
1	B	122	GLU	2.2
1	B	55	LYS	2.2
1	A	220	ARG	2.2
1	B	44	THR	2.1
1	B	53	GLU	2.1
1	A	186	ALA	2.1
1	B	38	LYS	2.0
1	B	414	LYS	2.0
1	A	518	ASN	2.0
2	P	1	DG	2.0
2	P	3	DG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	8OG	F	5	23/24	0.93	0.12	101,106,107,111	0
3	8OG	T	5	23/24	0.94	0.09	74,78,82,83	0

6.3 Carbohydrates [i](#)

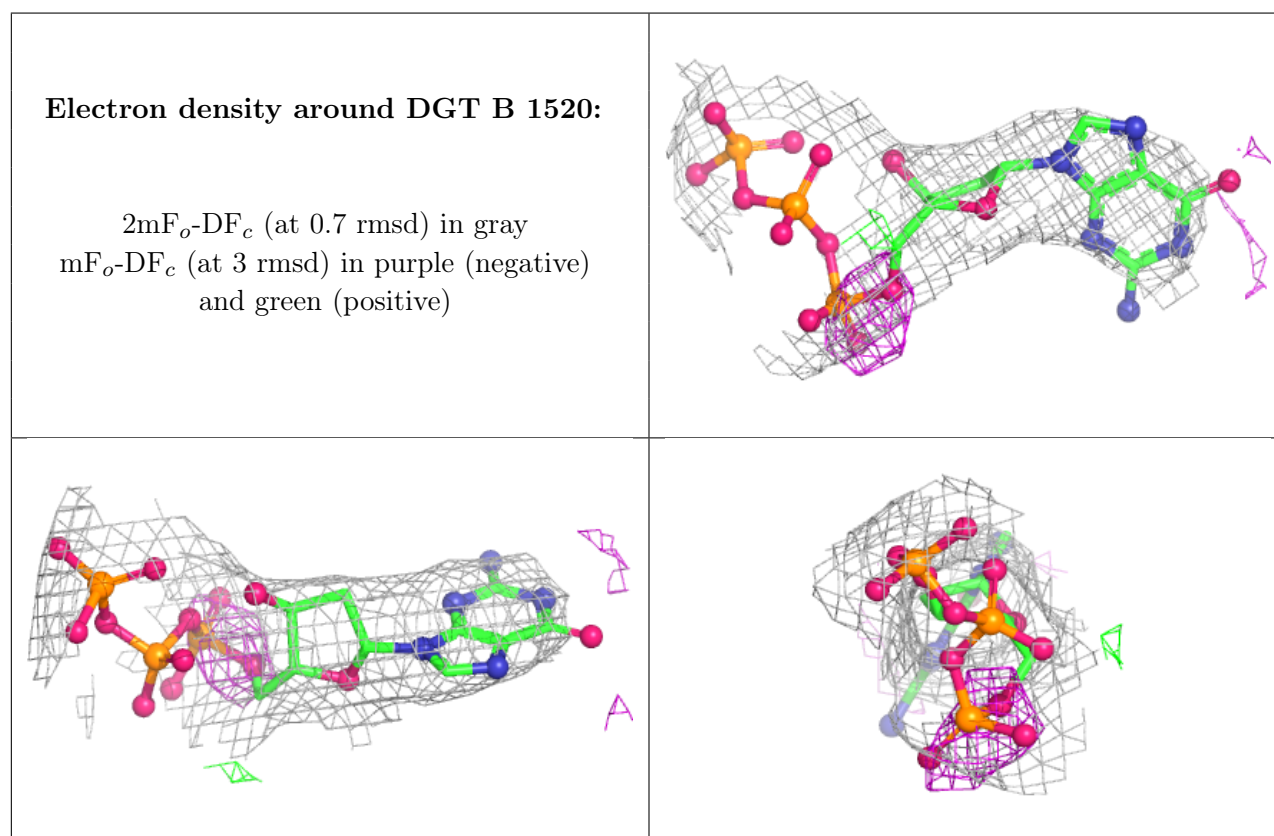
There are no oligosaccharides in this entry.

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.

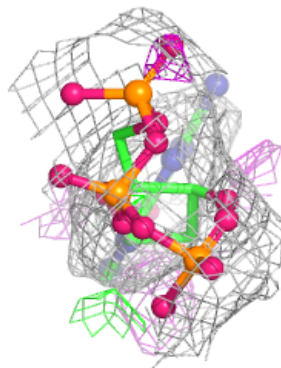
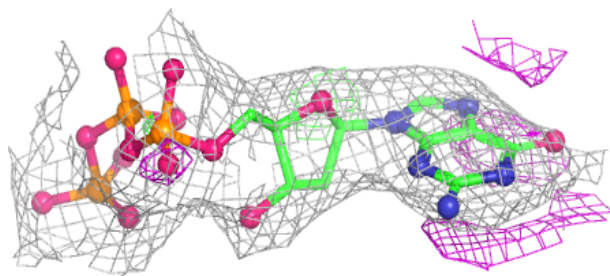
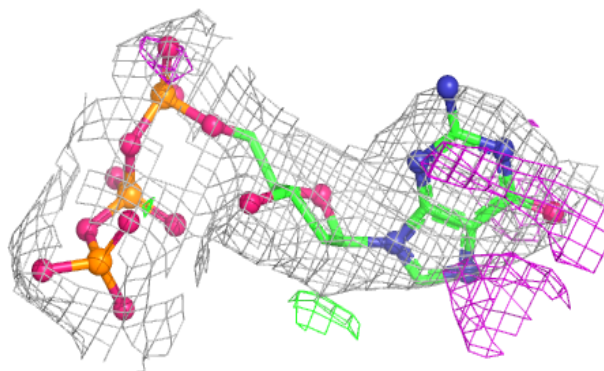
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DGT	B	1520	31/31	0.90	0.13	129,135,144,144	0
4	DGT	A	1520	31/31	0.94	0.12	74,87,103,106	0
5	CA	B	1521	1/1	0.97	0.08	117,117,117,117	0
5	CA	A	1521	1/1	0.98	0.04	60,60,60,60	0
5	CA	A	1522	1/1	0.99	0.08	63,63,63,63	0
5	CA	B	1522	1/1	0.99	0.04	95,95,95,95	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 DGT A 1520:

$2mF_o - DF_c$ (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.