



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 07:07 AM UTC

PDB ID : 4ZTU / pdb_00004ztu
Title : Structural basis for processivity and antiviral drug toxicity in human mitochondrial DNA replicase
Authors : Szymanski, M.R.; Kuznestov, V.B.; Shumate, C.K.; Meng, Q.; Lee, Y.-S.; Patel, G.; Patel, S.S.; Yin, Y.W.
Deposited on : 2015-05-15
Resolution : 3.30 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

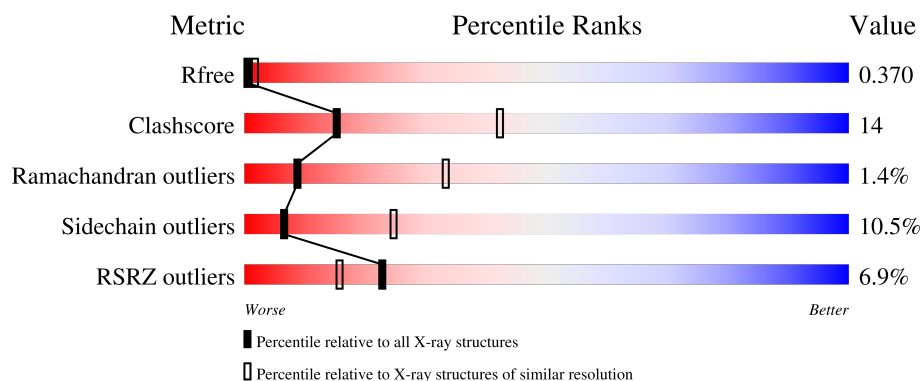
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1222	7% 53% 23% . 20%
2	B	472	5% 57% 17% . 23%
2	C	472	3% 55% 17% . 24%
3	T	27	7% 52% 41% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	P	24	 A horizontal bar chart showing the quality of chain 4. The bar is divided into three segments: a green segment representing 54%, a yellow segment representing 38%, and a grey segment representing 8%. The percentages are labeled below the bar.

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14619 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 subunit gamma-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	983	Total	C	N	O	S	0	0	0
			7799	4966	1371	1413	49			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	MET	-	expression tag	UNP P54098
A	198	ALA	ASP	engineered mutation	UNP P54098
A	200	ALA	GLU	engineered mutation	UNP P54098
A	1240	ALA	-	expression tag	UNP P54098
A	1241	ALA	-	expression tag	UNP P54098
A	1242	ALA	-	expression tag	UNP P54098
A	1243	LEU	-	expression tag	UNP P54098
A	1244	GLU	-	expression tag	UNP P54098
A	1245	HIS	-	expression tag	UNP P54098
A	1246	HIS	-	expression tag	UNP P54098
A	1247	HIS	-	expression tag	UNP P54098
A	1248	HIS	-	expression tag	UNP P54098
A	1249	HIS	-	expression tag	UNP P54098
A	1250	HIS	-	expression tag	UNP P54098

- Molecule 2 is a protein called DNA polymerase subunit gamma-2, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	363	Total	C	N	O	S	0	0	0
			2942	1885	520	521	16			
2	C	357	Total	C	N	O	S	0	0	0
			2886	1852	508	510	16			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	25	MET	-	expression tag	UNP Q9UHN1
B	486	ALA	-	expression tag	UNP Q9UHN1
B	487	ALA	-	expression tag	UNP Q9UHN1
B	488	ALA	-	expression tag	UNP Q9UHN1
B	489	LEU	-	expression tag	UNP Q9UHN1
B	490	GLU	-	expression tag	UNP Q9UHN1
B	491	HIS	-	expression tag	UNP Q9UHN1
B	492	HIS	-	expression tag	UNP Q9UHN1
B	493	HIS	-	expression tag	UNP Q9UHN1
B	494	HIS	-	expression tag	UNP Q9UHN1
B	495	HIS	-	expression tag	UNP Q9UHN1
B	496	HIS	-	expression tag	UNP Q9UHN1
C	25	MET	-	expression tag	UNP Q9UHN1
C	486	ALA	-	expression tag	UNP Q9UHN1
C	487	ALA	-	expression tag	UNP Q9UHN1
C	488	ALA	-	expression tag	UNP Q9UHN1
C	489	LEU	-	expression tag	UNP Q9UHN1
C	490	GLU	-	expression tag	UNP Q9UHN1
C	491	HIS	-	expression tag	UNP Q9UHN1
C	492	HIS	-	expression tag	UNP Q9UHN1
C	493	HIS	-	expression tag	UNP Q9UHN1
C	494	HIS	-	expression tag	UNP Q9UHN1
C	495	HIS	-	expression tag	UNP Q9UHN1
C	496	HIS	-	expression tag	UNP Q9UHN1

- Molecule 3 is a DNA chain called DNA (25-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	25	Total	C	N	O	P	0	0	0
			508	241	89	153	25			

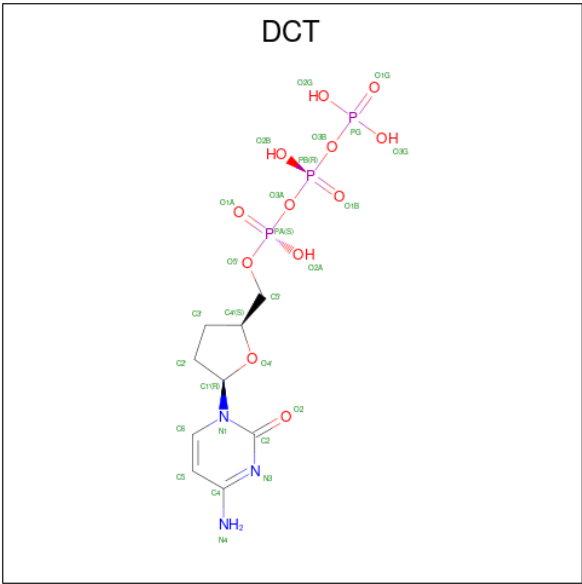
- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*AP*GP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	22	Total	C	N	O	P	0	0	0
			455	214	92	127	22			

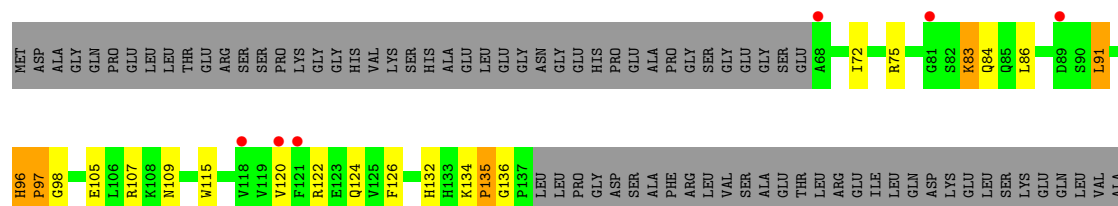
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

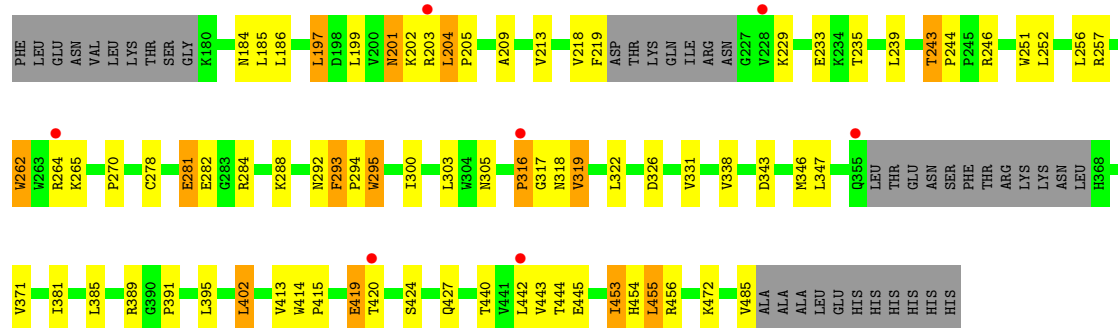
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 2',3'-DIDEOXYCYTIDINE 5'-TRIPHOSPHATE (CCD ID: DCT) (formula: $C_9H_{16}N_3O_{12}P_3$).

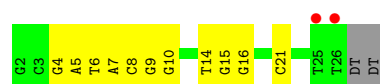


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	27	9	3	12	3	0	0

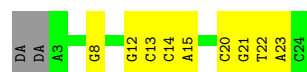




• Molecule 3: DNA (25-MER)



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	217.57Å 217.57Å 168.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.67 – 3.30 42.67 – 3.30	Depositor EDS
% Data completeness (in resolution range)	98.8 (42.67-3.30) 85.7 (42.67-3.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.33Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.316 , 0.316 0.354 , 0.370	Depositor DCC
R_{free} test set	2000 reflections (3.29%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 19.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14619	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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: MG, DCT, DOC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.31	0/7999	0.77	11/10852 (0.1%)
2	B	0.25	0/3015	0.70	0/4074
2	C	0.27	0/2959	0.75	4/4000 (0.1%)
3	T	0.18	0/567	0.33	0/872
4	P	0.16	0/492	0.27	0/758
All	All	0.28	0/15032	0.73	15/20556 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	PRO	CA-N-CD	-8.94	99.49	112.00
2	C	96	HIS	C-N-CD	-8.37	102.19	120.60
1	A	752	LEU	CA-C-N	6.48	142.56	127.00
1	A	752	LEU	C-N-CA	6.48	142.56	127.00
1	A	1089	GLN	N-CA-C	6.36	118.74	111.11
1	A	752	LEU	C-N-CD	-6.27	106.81	120.60
2	C	96	HIS	CA-C-N	6.04	141.49	127.00
2	C	96	HIS	C-N-CA	6.04	141.49	127.00
1	A	635	PRO	N-CA-C	5.94	119.54	111.22
1	A	1054	GLU	CB-CA-C	-5.86	109.27	117.23
1	A	634	LEU	CA-C-N	5.30	125.30	120.21
1	A	634	LEU	C-N-CA	5.30	125.30	120.21
1	A	1069	ILE	CA-C-N	5.22	126.37	119.84
1	A	1069	ILE	C-N-CA	5.22	126.37	119.84
1	A	633	LYS	N-CA-C	5.20	117.58	109.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7799	0	7696	247	0
2	B	2942	0	2939	60	0
2	C	2886	0	2874	79	0
3	T	508	0	282	16	0
4	P	455	0	245	10	0
5	A	2	0	0	0	0
6	A	27	0	12	2	0
All	All	14619	0	14048	389	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 14.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:CD2	1:A:635:PRO:HD2	1.37	1.49
1:A:634:LEU:HD23	1:A:635:PRO:CD	1.39	1.49
1:A:631:LEU:C	1:A:633:LYS:CE	1.95	1.32
1:A:631:LEU:C	1:A:633:LYS:HE2	1.38	1.29
1:A:640:LEU:C	1:A:640:LEU:HD22	1.61	1.25
1:A:632:ALA:C	1:A:633:LYS:HD3	1.62	1.24
1:A:640:LEU:HD22	1:A:640:LEU:O	1.41	1.18
2:B:418:LEU:O	2:C:203:ARG:NH1	1.76	1.17
1:A:631:LEU:O	1:A:633:LYS:HE2	1.44	1.11
2:C:135:PRO:HD2	2:C:136:GLY:H	1.10	1.11
2:C:134:LYS:CD	2:C:135:PRO:HD3	1.79	1.10
1:A:641:GLU:HG3	1:A:642:SER:N	1.57	1.08
1:A:632:ALA:N	1:A:633:LYS:HE2	1.71	1.06
1:A:641:GLU:HG3	1:A:642:SER:H	1.09	1.01
2:C:134:LYS:HD2	2:C:135:PRO:CD	1.92	1.00
2:C:134:LYS:HD2	2:C:135:PRO:HD3	1.00	0.99
1:A:640:LEU:C	1:A:640:LEU:CD2	2.36	0.97
1:A:632:ALA:O	1:A:633:LYS:HD3	1.66	0.95
2:C:419:GLU:H	2:C:420:THR:HA	1.32	0.93
1:A:649:TYR:CB	1:A:750:PHE:CZ	2.54	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ALA:C	1:A:633:LYS:CD	2.45	0.88
2:C:134:LYS:NZ	2:C:135:PRO:HD2	1.89	0.87
1:A:1068:ASP:HA	1:A:1085:PRO:HG2	1.56	0.86
1:A:632:ALA:N	1:A:633:LYS:CE	2.35	0.85
2:C:135:PRO:HD2	2:C:136:GLY:N	1.87	0.84
1:A:849:THR:HG22	1:A:850:ILE:HD13	1.57	0.83
1:A:631:LEU:O	1:A:633:LYS:CE	2.11	0.82
2:C:134:LYS:CD	2:C:135:PRO:CD	2.54	0.80
1:A:649:TYR:CB	1:A:750:PHE:CE2	2.65	0.79
1:A:641:GLU:CG	1:A:642:SER:N	2.44	0.78
2:C:134:LYS:HZ3	2:C:135:PRO:CD	1.98	0.77
1:A:641:GLU:O	1:A:642:SER:HB3	1.84	0.77
1:A:632:ALA:CA	1:A:633:LYS:HE2	2.14	0.76
2:C:135:PRO:CD	2:C:136:GLY:H	1.93	0.76
2:C:442:LEU:HB3	2:C:454:HIS:HB2	1.67	0.76
1:A:630:ASN:C	1:A:631:LEU:HD23	2.11	0.75
1:A:744:ILE:HG23	1:A:745:PRO:HD3	1.68	0.75
2:B:444:THR:HG22	2:B:447:THR:HG23	1.71	0.72
1:A:800:PHE:HB2	1:A:869:ARG:HE	1.53	0.72
1:A:640:LEU:O	1:A:640:LEU:CD2	2.30	0.72
1:A:633:LYS:HD3	1:A:633:LYS:N	1.95	0.71
1:A:634:LEU:HD23	1:A:635:PRO:HD3	1.65	0.71
2:C:134:LYS:NZ	2:C:135:PRO:CD	2.54	0.71
1:A:631:LEU:HD23	1:A:631:LEU:N	2.04	0.70
1:A:487:ASP:OD2	1:A:601:LYS:NZ	2.24	0.70
1:A:243:ASP:HB3	1:A:279:ARG:HE	1.57	0.69
1:A:153:ALA:HB1	1:A:194:ALA:HB2	1.74	0.68
1:A:1057:MET:SD	1:A:1057:MET:N	2.64	0.68
1:A:634:LEU:HD22	1:A:635:PRO:HD2	1.67	0.68
2:C:134:LYS:HZ3	2:C:135:PRO:HD2	1.55	0.67
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.77	0.66
2:B:197:LEU:HD22	2:B:202:LYS:HA	1.76	0.66
1:A:464:MET:HB2	1:A:589:PRO:HG2	1.78	0.66
1:A:211:LEU:HD22	1:A:393:MET:HE2	1.77	0.66
1:A:850:ILE:HG22	3:T:6:DT:H4'	1.76	0.66
1:A:896:LEU:HD21	1:A:931:LEU:HD23	1.77	0.66
1:A:1108:TYR:OH	1:A:1161:ARG:NH1	2.24	0.66
1:A:533:CYS:SG	1:A:534:SER:N	2.68	0.65
1:A:963:GLU:HA	1:A:981:LYS:HE2	1.78	0.65
1:A:1096:ARG:HA	1:A:1099:TRP:HB3	1.79	0.65
2:C:443:VAL:HG22	2:C:453:ILE:HD11	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.78	0.64
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.77	0.64
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.79	0.64
1:A:642:SER:OG	1:A:643:ALA:HA	1.98	0.63
3:T:21:DC:H42	4:P:8:DG:H1	1.46	0.63
1:A:502:LYS:HB3	1:A:503:VAL:HB	1.80	0.62
1:A:606:THR:HG22	1:A:612:LEU:HD22	1.81	0.62
1:A:642:SER:OG	1:A:643:ALA:CA	2.47	0.62
1:A:921:LEU:HD22	1:A:1174:PRO:HG2	1.82	0.62
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.64	0.62
2:C:265:LYS:CD	2:C:485:VAL:HG22	2.29	0.62
2:C:419:GLU:N	2:C:420:THR:HA	2.05	0.62
1:A:633:LYS:CD	1:A:633:LYS:N	2.56	0.62
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.82	0.61
2:B:382:LYS:H	2:B:412:SER:HB2	1.65	0.61
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.82	0.61
2:C:292:ASN:HD21	2:C:294:PRO:HB3	1.65	0.61
1:A:899:ALA:HB1	1:A:1057:MET:HE3	1.82	0.60
2:C:219:PHE:HD1	2:C:229:LYS:HG2	1.66	0.60
2:B:77:HIS:NE2	2:B:434:GLU:OE2	2.35	0.60
2:B:441:VAL:HG23	2:B:453:ILE:HG13	1.84	0.60
2:B:363:ARG:HD3	2:B:364:LYS:H	1.66	0.60
2:B:104:VAL:HG23	2:B:107:ARG:HH21	1.66	0.60
2:C:134:LYS:HZ2	2:C:135:PRO:HD2	1.67	0.60
1:A:79:LEU:H	1:A:83:LEU:HG	1.66	0.59
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.59
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.84	0.59
2:C:135:PRO:CD	2:C:136:GLY:N	2.55	0.59
1:A:558:LEU:HD13	1:A:559:LEU:HD12	1.85	0.59
1:A:911:HIS:NE2	1:A:1172:ASP:O	2.36	0.59
1:A:463:LEU:HB3	1:A:592:LEU:HD12	1.85	0.58
1:A:593:SER:HB2	1:A:596:MET:HB2	1.84	0.58
1:A:887:VAL:HG22	1:A:1185:ILE:HG23	1.84	0.58
1:A:978:ALA:HA	1:A:981:LYS:HD2	1.85	0.58
2:B:77:HIS:HE1	2:B:431:LYS:HG3	1.66	0.58
3:T:16:DG:H1	4:P:13:DC:H42	1.51	0.58
2:B:241:TRP:HB3	2:B:336:LEU:HB3	1.84	0.58
1:A:804:ALA:HB1	1:A:808:ILE:HD11	1.85	0.58
1:A:1069:ILE:HB	1:A:1070:PRO:HD2	1.85	0.58
1:A:831:TYR:H	1:A:832:ASP:HA	1.69	0.58
2:B:117:SER:O	2:B:122:ARG:NH1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:LEU:HD23	1:A:635:PRO:HD2	0.63	0.57
1:A:938:THR:H	1:A:939:VAL:HA	1.69	0.57
1:A:1161:ARG:HE	1:A:1177:VAL:HG22	1.69	0.57
1:A:1133:ILE:HG12	1:A:1136:GLU:HB3	1.85	0.57
1:A:208:CYS:SG	1:A:227:ARG:NH2	2.78	0.57
2:C:246:ARG:NH2	2:C:326:ASP:OD2	2.38	0.57
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.38	0.57
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.87	0.56
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.87	0.56
1:A:825:VAL:HG13	1:A:882:PRO:HG2	1.86	0.56
2:B:444:THR:HG23	2:B:446:THR:H	1.69	0.56
1:A:245:ILE:HG13	1:A:289:MET:HE3	1.88	0.56
1:A:200:ALA:HB3	1:A:211:LEU:HB2	1.88	0.56
1:A:632:ALA:N	1:A:633:LYS:NZ	2.42	0.56
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.88	0.56
2:B:252:LEU:HD13	2:B:336:LEU:HD11	1.87	0.56
2:C:381:ILE:HG21	2:C:414:TRP:HB2	1.87	0.56
1:A:647:CYS:SG	1:A:648:PRO:HD2	2.46	0.56
2:B:407:LEU:HD13	2:C:120:VAL:HG12	1.87	0.56
1:A:851:THR:O	1:A:851:THR:OG1	2.24	0.55
2:C:134:LYS:HG3	2:C:135:PRO:HD2	1.87	0.55
1:A:239:LEU:O	1:A:279:ARG:NH1	2.40	0.55
1:A:1089:GLN:N	1:A:1090:GLU:HA	2.21	0.55
2:C:134:LYS:CG	2:C:135:PRO:CD	2.84	0.55
2:B:446:THR:O	2:B:450:ASN:ND2	2.40	0.55
2:C:107:ARG:HB2	2:C:346:MET:HE2	1.87	0.55
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.22	0.55
2:B:457:SER:OG	2:B:460:THR:O	2.25	0.54
1:A:107:LEU:O	1:A:112:LEU:N	2.35	0.54
2:B:428:LEU:HD13	2:B:428:LEU:H	1.71	0.54
2:C:96:HIS:HB3	2:C:97:PRO:C	2.32	0.54
1:A:647:CYS:SG	1:A:648:PRO:CD	2.96	0.54
1:A:1124:ALA:O	1:A:1148:ARG:NH2	2.40	0.54
2:B:418:LEU:HD22	2:C:204:LEU:HD12	1.90	0.54
1:A:755:LYS:HD2	1:A:758:ASN:HD22	1.73	0.54
1:A:1142:ARG:NH1	1:A:1144:GLU:OE1	2.37	0.53
2:C:262:TRP:HA	2:C:265:LYS:HE2	1.90	0.53
2:C:444:THR:OG1	2:C:445:GLU:N	2.36	0.53
1:A:803:ASN:HA	3:T:10:DG:H4'	1.89	0.53
1:A:566:LEU:HD13	1:A:566:LEU:H	1.73	0.53
2:C:319:VAL:HA	2:C:322:LEU:HD13	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:869:ARG:NH1	4:P:22:DT:OP1	2.42	0.53
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.91	0.53
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.90	0.53
1:A:864:ASN:O	1:A:872:SER:OG	2.25	0.53
1:A:353:VAL:HG13	1:A:355:SER:H	1.74	0.53
2:B:393:LEU:HD12	2:B:394:GLU:HG2	1.90	0.53
2:C:389:ARG:HD3	2:C:395:LEU:HD11	1.91	0.52
2:C:205:PRO:HB3	2:C:244:PRO:HD3	1.92	0.52
1:A:895:GLU:OE1	1:A:955:TYR:OH	2.28	0.52
1:A:861:THR:HG21	3:T:8:DC:H1'	1.91	0.52
2:B:185:LEU:H	2:B:185:LEU:HD23	1.74	0.52
1:A:639:THR:HG22	1:A:640:LEU:N	2.25	0.52
1:A:865:ALA:H	1:A:1191:LYS:HD3	1.75	0.52
1:A:1072:THR:O	1:A:1072:THR:OG1	2.20	0.52
1:A:642:SER:OG	1:A:643:ALA:HB2	2.09	0.52
1:A:631:LEU:N	1:A:631:LEU:CD2	2.72	0.51
1:A:647:CYS:SG	1:A:648:PRO:N	2.83	0.51
1:A:894:GLN:HG3	1:A:895:GLU:H	1.75	0.51
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.92	0.51
1:A:384:ASP:OD1	1:A:384:ASP:N	2.40	0.51
1:A:743:ASP:OD1	1:A:743:ASP:N	2.35	0.51
1:A:1183:VAL:N	1:A:1214:GLN:O	2.44	0.51
2:C:134:LYS:HG3	2:C:135:PRO:CD	2.41	0.51
1:A:176:THR:OG1	1:A:222:SER:OG	2.26	0.51
1:A:634:LEU:CG	1:A:635:PRO:HD2	2.31	0.51
1:A:850:ILE:HD12	1:A:851:THR:HA	1.92	0.51
1:A:93:GLU:HA	1:A:94:MET:HB2	1.93	0.51
1:A:211:LEU:HD12	1:A:377:PHE:HZ	1.76	0.50
1:A:272:SER:HB3	1:A:843:GLN:HA	1.93	0.50
1:A:1069:ILE:O	1:A:1071:ARG:N	2.44	0.50
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.84	0.50
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.47	0.50
1:A:175:TRP:CD2	1:A:223:TRP:HB2	2.45	0.50
1:A:296:SER:HB2	1:A:847:ALA:HB3	1.93	0.50
1:A:641:GLU:O	1:A:642:SER:CB	2.55	0.50
1:A:1032:THR:O	1:A:1034:ARG:NH2	2.44	0.50
1:A:639:THR:HG22	1:A:640:LEU:H	1.77	0.50
3:T:14:DT:H2''	3:T:15:DG:C8	2.47	0.50
1:A:641:GLU:OE1	1:A:642:SER:O	2.30	0.50
1:A:617:ARG:HB2	1:A:763:GLY:HA3	1.94	0.50
1:A:1075:LEU:HD23	1:A:1075:LEU:H	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:GLN:HE22	2:C:203:ARG:NH2	2.09	0.50
2:C:264:ARG:HG3	2:C:270:PRO:HB3	1.92	0.50
2:C:252:LEU:HD22	2:C:305:ASN:HB2	1.93	0.50
1:A:298:HIS:HD2	1:A:363:TYR:HE1	1.60	0.49
1:A:546:ARG:NH2	2:B:408:GLU:OE2	2.44	0.49
1:A:488:LEU:HD13	1:A:488:LEU:H	1.77	0.49
2:C:205:PRO:HB3	2:C:243:THR:HA	1.94	0.49
1:A:606:THR:HB	1:A:612:LEU:HD13	1.95	0.49
4:P:14:DC:H2'	4:P:15:DA:C8	2.48	0.49
1:A:622:TYR:HB2	1:A:770:PHE:HE2	1.76	0.49
1:A:887:VAL:HG13	1:A:1185:ILE:HG12	1.93	0.49
1:A:136:ASP:HA	1:A:1163:MET:HE1	1.95	0.49
1:A:630:ASN:OD1	1:A:630:ASN:O	2.30	0.49
1:A:770:PHE:HB3	1:A:773:LYS:HB3	1.95	0.49
1:A:562:ARG:HD2	1:A:563:PRO:HD2	1.95	0.49
1:A:1108:TYR:HE1	1:A:1161:ARG:HD3	1.77	0.49
1:A:134:ASN:ND2	1:A:1166:TYR:OH	2.37	0.48
3:T:9:DG:H2'	3:T:10:DG:C8	2.47	0.48
1:A:616:GLU:HB2	1:A:617:ARG:HD3	1.96	0.48
1:A:593:SER:C	1:A:596:MET:H	2.21	0.48
2:B:388:GLY:HA3	2:B:442:LEU:HD11	1.94	0.48
2:C:134:LYS:HZ3	2:C:135:PRO:CG	2.25	0.48
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.95	0.48
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.94	0.48
1:A:632:ALA:C	1:A:633:LYS:CE	2.87	0.48
2:B:213:VAL:HA	2:B:235:THR:HA	1.96	0.48
1:A:536:GLU:HG3	2:C:257:ARG:HH12	1.78	0.48
2:B:219:PHE:HA	2:B:229:LYS:N	2.29	0.48
2:B:404:ASN:HA	2:B:407:LEU:HG	1.95	0.48
1:A:761:ASN:OD1	1:A:761:ASN:N	2.47	0.48
1:A:1187:ARG:HH11	1:A:1209:ARG:HH12	1.61	0.48
1:A:91:GLY:HA2	1:A:92:GLY:HA3	1.58	0.48
1:A:357:ALA:HA	1:A:369:LEU:HD21	1.96	0.48
1:A:631:LEU:O	1:A:633:LYS:HE3	2.10	0.48
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.48	0.48
1:A:955:TYR:CE2	3:T:4:DG:N2	2.82	0.47
1:A:1200:PRO:O	1:A:1202:ASN:N	2.43	0.47
1:A:645:VAL:O	1:A:645:VAL:CG1	2.60	0.47
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.95	0.47
1:A:1068:ASP:OD2	1:A:1068:ASP:N	2.46	0.47
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:PHE:HB3	2:C:295:TRP:H	1.79	0.47
1:A:299:MET:HE3	1:A:848:GLY:HA2	1.96	0.47
3:T:4:DG:C2	3:T:5:DA:C4	3.02	0.47
1:A:491:ASP:HB2	1:A:574:ARG:HH12	1.80	0.47
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.71	0.47
1:A:955:TYR:CE1	1:A:1101:VAL:HG11	2.49	0.47
2:B:420:THR:HG23	2:B:421:MET:HG2	1.97	0.47
1:A:135:LEU:HD23	1:A:135:LEU:H	1.80	0.47
1:A:480:LYS:HD3	1:A:646:VAL:HG11	1.96	0.47
1:A:612:LEU:HD12	1:A:612:LEU:HA	1.83	0.47
2:C:265:LYS:HD2	2:C:485:VAL:HG22	1.97	0.47
1:A:1069:ILE:CB	1:A:1070:PRO:HD2	2.45	0.47
1:A:304:LEU:HD13	1:A:309:ARG:HG2	1.96	0.46
1:A:976:GLN:O	1:A:980:GLU:HG2	2.15	0.46
2:C:303:LEU:HD22	2:C:338:VAL:HG22	1.98	0.46
1:A:642:SER:OG	1:A:643:ALA:CB	2.64	0.46
1:A:782:GLY:HA2	1:A:784:GLY:HA2	1.98	0.46
1:A:1115:ALA:HB3	1:A:1156:THR:HG23	1.97	0.46
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.55	0.46
2:B:78:PHE:HD2	2:C:199:LEU:HD13	1.79	0.46
4:P:22:DT:H2'	4:P:23:DA:C8	2.50	0.46
2:B:363:ARG:O	2:B:364:LYS:HG3	2.15	0.46
2:C:91:LEU:HD12	2:C:347:LEU:HD21	1.97	0.46
1:A:178:TYR:O	1:A:219:ALA:HB1	2.16	0.46
2:B:402:LEU:HD13	2:B:468:ILE:HG23	1.98	0.46
1:A:640:LEU:HD22	1:A:641:GLU:N	2.24	0.46
3:T:21:DC:N4	4:P:8:DG:H1	2.13	0.46
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.98	0.46
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.51	0.46
1:A:942:SER:HA	1:A:943:ARG:HA	1.59	0.46
1:A:1060:LYS:O	1:A:1064:ILE:HG12	2.16	0.46
1:A:298:HIS:HB2	1:A:410:GLN:HE22	1.79	0.45
1:A:634:LEU:CD2	1:A:635:PRO:CD	2.30	0.45
1:A:778:THR:HA	1:A:779:LEU:HA	1.60	0.45
1:A:599:THR:HA	1:A:602:LEU:HB3	1.99	0.45
2:C:201:ASN:HB3	2:C:203:ARG:HG3	1.98	0.45
1:A:741:ASP:HB3	1:A:745:PRO:HB2	1.98	0.45
1:A:1135:ASP:HB2	6:A:4003:DCT:H5''	1.99	0.45
1:A:765:PRO:HA	1:A:766:PHE:HA	1.58	0.45
1:A:869:ARG:HB2	1:A:872:SER:HB2	1.98	0.45
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.81	0.45
2:C:72:ILE:HA	2:C:75:ARG:HG2	1.97	0.45
2:C:239:LEU:HB3	2:C:338:VAL:HB	1.98	0.45
2:C:105:GLU:O	2:C:109:ASN:ND2	2.47	0.45
2:C:316:PRO:HA	2:C:317:GLY:HA2	1.48	0.45
1:A:594:LEU:N	1:A:596:MET:H	2.15	0.45
1:A:1157:ASN:ND2	1:A:1178:ALA:O	2.49	0.45
2:C:440:THR:OG1	2:C:456:ARG:HB3	2.16	0.45
1:A:309:ARG:NH2	1:A:849:THR:OG1	2.49	0.45
2:B:75:ARG:NH1	2:B:84:GLN:OE1	2.50	0.45
2:B:101:PRO:HB3	2:C:126:PHE:HB3	1.98	0.45
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.60	0.45
2:C:414:TRP:HA	2:C:415:PRO:HD3	1.88	0.45
1:A:495:PHE:HB3	1:A:496:LYS:HD3	1.98	0.45
1:A:570:PRO:HB2	1:A:572:TRP:CD1	2.52	0.44
1:A:955:TYR:CD2	3:T:4:DG:N2	2.85	0.44
2:B:200:VAL:HG13	2:B:203:ARG:H	1.82	0.44
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.99	0.44
2:B:133:HIS:ND1	2:C:233:GLU:OE2	2.50	0.44
2:B:421:MET:HA	2:B:422:GLN:HB3	2.00	0.44
1:A:556:THR:HA	1:A:559:LEU:HD13	1.99	0.44
1:A:239:LEU:HD13	1:A:239:LEU:HA	1.85	0.44
1:A:642:SER:CB	1:A:643:ALA:HA	2.43	0.44
1:A:645:VAL:O	1:A:645:VAL:HG12	2.17	0.44
1:A:646:VAL:CG2	1:A:647:CYS:N	2.79	0.44
2:C:265:LYS:HD3	2:C:485:VAL:HG22	1.98	0.44
1:A:475:SER:HA	1:A:476:GLY:HA2	1.50	0.44
1:A:987:ALA:HB1	1:A:1056:GLU:HG2	1.99	0.44
2:B:79:LEU:HG	2:B:102:LEU:HB2	2.00	0.44
2:B:467:HIS:HB3	2:B:470:LYS:HB2	1.99	0.44
1:A:79:LEU:HD13	1:A:80:SER:H	1.83	0.44
1:A:276:ALA:O	1:A:282:TYR:OH	2.30	0.44
1:A:497:GLN:NE2	1:A:559:LEU:HB3	2.32	0.44
1:A:582:ASP:HA	1:A:583:PRO:HD3	1.91	0.44
1:A:1079:ILE:H	1:A:1079:ILE:HG13	1.70	0.44
2:B:365:LYS:HG2	2:B:367:LEU:H	1.83	0.44
2:B:372:LEU:HD13	2:B:436:SER:HB2	1.99	0.44
1:A:973:LEU:HD22	1:A:976:GLN:H	1.83	0.43
4:P:22:DT:H2'	4:P:23:DA:H8	1.83	0.43
1:A:1154:GLN:HG3	1:A:1218:LEU:HD21	1.99	0.43
2:B:365:LYS:H	2:B:365:LYS:HD2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:134:LYS:CE	2:C:135:PRO:HD3	2.47	0.43
1:A:307:PHE:O	1:A:310:SER:OG	2.36	0.43
1:A:856:GLU:N	1:A:860:LEU:HD12	2.33	0.43
1:A:1079:ILE:HG12	1:A:1099:TRP:CE3	2.53	0.43
1:A:1080:SER:OG	1:A:1083:LEU:HB2	2.19	0.43
2:B:447:THR:HG21	2:B:453:ILE:HA	2.00	0.43
1:A:299:MET:HG3	1:A:849:THR:HG23	2.01	0.43
3:T:6:DT:H2'	3:T:7:DA:O4'	2.18	0.43
1:A:963:GLU:HG3	1:A:981:LYS:NZ	2.33	0.43
2:C:209:ALA:HB2	2:C:239:LEU:HD13	1.99	0.43
2:C:292:ASN:ND2	2:C:294:PRO:HB3	2.32	0.43
1:A:807:ARG:HD3	3:T:9:DG:H4'	2.00	0.43
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.53	0.43
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.88	0.43
1:A:298:HIS:CD2	1:A:363:TYR:HE1	2.36	0.43
1:A:549:LEU:HD11	2:B:468:ILE:HG21	1.99	0.43
1:A:892:ASP:HA	1:A:893:SER:HA	1.66	0.43
1:A:950:ASN:O	1:A:954:ILE:HG13	2.18	0.43
2:C:124:GLN:HE22	2:C:203:ARG:HH21	1.67	0.43
1:A:865:ALA:HB2	1:A:1191:LYS:HZ2	1.84	0.43
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	2.00	0.42
1:A:567:PRO:HA	1:A:574:ARG:HE	1.84	0.42
1:A:856:GLU:OE1	1:A:859:TRP:N	2.36	0.42
1:A:891:VAL:HG13	1:A:1161:ARG:HH12	1.83	0.42
2:B:303:LEU:HG	2:B:338:VAL:HB	2.01	0.42
2:C:265:LYS:HD3	2:C:485:VAL:CG2	2.48	0.42
4:P:20:DC:H2''	4:P:21:DG:C8	2.54	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.90	0.42
1:A:594:LEU:HA	1:A:595:GLN:HA	1.85	0.42
1:A:749:PHE:HB2	1:A:750:PHE:H	1.59	0.42
2:B:83:LYS:HG2	2:B:85:GLN:H	1.84	0.42
3:T:4:DG:N3	3:T:5:DA:C8	2.87	0.42
1:A:608:ASP:OD1	1:A:778:THR:OG1	2.26	0.42
1:A:1108:TYR:CE1	1:A:1161:ARG:HD3	2.54	0.42
2:C:134:LYS:HZ3	2:C:135:PRO:HG2	1.83	0.42
1:A:622:TYR:HB2	1:A:770:PHE:CE2	2.54	0.42
1:A:850:ILE:CG1	1:A:851:THR:HA	2.49	0.42
2:C:184:ASN:OD1	2:C:185:LEU:N	2.44	0.42
2:C:455:LEU:HD23	2:C:455:LEU:HA	1.90	0.42
1:A:977:GLU:HB3	1:A:981:LYS:NZ	2.35	0.42
2:C:126:PHE:CE2	2:C:199:LEU:HB3	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLY:HA2	1:A:532:PRO:HD3	1.84	0.42
2:B:423:SER:OG	2:B:424:SER:N	2.53	0.42
2:B:439:PHE:HB3	2:B:455:LEU:HD11	2.01	0.42
2:C:293:PHE:N	2:C:294:PRO:HA	2.35	0.41
1:A:579:ARG:NH1	4:P:12:DG:OP1	2.53	0.41
1:A:856:GLU:HA	1:A:857:PRO:HD3	1.88	0.41
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.92	0.41
2:C:281:GLU:CD	2:C:281:GLU:H	2.27	0.41
1:A:556:THR:HB	2:B:467:HIS:NE2	2.35	0.41
2:B:364:LYS:HB2	2:B:364:LYS:HE2	1.63	0.41
2:C:134:LYS:CE	2:C:135:PRO:CD	2.98	0.41
1:A:607:TRP:HA	1:A:778:THR:HG23	2.01	0.41
2:B:384:ALA:HB2	2:B:437:ILE:HD13	2.01	0.41
1:A:298:HIS:HB2	1:A:410:GLN:NE2	2.35	0.41
1:A:505:LYS:HA	1:A:505:LYS:HD3	1.76	0.41
1:A:860:LEU:HD23	1:A:1133:ILE:HG22	2.02	0.41
1:A:170:ALA:HB3	1:A:176:THR:HG21	2.03	0.41
6:A:4003:DCT:N3	3:T:4:DG:N1	2.61	0.41
2:C:472:LYS:HE2	2:C:472:LYS:HB3	1.91	0.41
2:B:213:VAL:HG11	2:C:132:HIS:CE1	2.55	0.41
1:A:110:HIS:HB3	1:A:111:GLY:HA2	2.01	0.41
1:A:593:SER:HB3	1:A:594:LEU:C	2.45	0.41
1:A:606:THR:HG21	1:A:612:LEU:N	2.36	0.41
1:A:953:ARG:HG3	1:A:957:ALA:HB2	2.02	0.41
1:A:961:PHE:O	1:A:964:ARG:HD2	2.20	0.41
1:A:356:LEU:HA	1:A:359:VAL:HG12	2.02	0.41
1:A:828:HIS:CG	1:A:829:PRO:HD2	2.55	0.41
1:A:1198:LYS:HB3	1:A:1198:LYS:HE3	1.84	0.41
2:B:385:LEU:HA	2:B:441:VAL:HG13	2.03	0.41
2:B:393:LEU:HA	2:B:394:GLU:HA	1.65	0.41
1:A:142:LEU:HD22	1:A:1118:TRP:HB2	2.02	0.40
1:A:632:ALA:C	1:A:633:LYS:HE2	2.44	0.40
1:A:641:GLU:CG	1:A:642:SER:H	2.01	0.40
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.87	0.40
2:C:385:LEU:HD22	2:C:402:LEU:HD13	2.03	0.40
3:T:16:DG:H1	4:P:13:DC:N4	2.17	0.40
1:A:97:GLU:HA	1:A:100:VAL:HG22	2.03	0.40
2:C:284:ARG:CZ	2:C:284:ARG:HA	2.51	0.40
1:A:850:ILE:HD12	1:A:850:ILE:HA	1.86	0.40
1:A:1025:LEU:HB3	1:A:1026:ARG:H	1.68	0.40
2:B:70:LEU:HD23	2:B:70:LEU:H	1.86	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	969/1222 (79%)	846 (87%)	106 (11%)	17 (2%)	6	29
2	B	355/472 (75%)	326 (92%)	27 (8%)	2 (1%)	21	52
2	C	349/472 (74%)	326 (93%)	18 (5%)	5 (1%)	9	33
All	All	1673/2166 (77%)	1498 (90%)	151 (9%)	24 (1%)	9	33

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	LEU
1	A	1070	PRO
2	C	97	PRO
1	A	648	PRO
1	A	767	ALA
1	A	811	GLN
1	A	1073	PRO
1	A	1080	SER
1	A	1177	VAL
2	C	98	GLY
1	A	95	PRO
1	A	749	PHE
1	A	927	ARG
2	B	461	THR
1	A	642	SER
1	A	765	PRO
1	A	1074	VAL
1	A	1207	GLU
2	C	316	PRO
2	C	319	VAL
2	C	391	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	755	LYS
2	B	451	GLY
1	A	1141	VAL

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	823/1029 (80%)	718 (87%)	105 (13%)	4	18
2	B	325/415 (78%)	302 (93%)	23 (7%)	13	40
2	C	318/415 (77%)	292 (92%)	26 (8%)	10	35
All	All	1466/1859 (79%)	1312 (90%)	154 (10%)	6	25

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	93	GLU
1	A	101	ARG
1	A	118	VAL
1	A	123	VAL
1	A	130	LEU
1	A	195	LEU
1	A	196	VAL
1	A	201	VAL
1	A	227	ARG
1	A	236	THR
1	A	245	ILE
1	A	247	LEU
1	A	264	GLN
1	A	292	LEU
1	A	304	LEU
1	A	311	LEU
1	A	316	LYS
1	A	342	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	346	ASP
1	A	376	LEU
1	A	411	LEU
1	A	424	LEU
1	A	473	LEU
1	A	485	LEU
1	A	488	LEU
1	A	489	GLU
1	A	496	LYS
1	A	499	LYS
1	A	542	ASP
1	A	543	VAL
1	A	548	CYS
1	A	558	LEU
1	A	565	HIS
1	A	566	LEU
1	A	595	GLN
1	A	602	LEU
1	A	612	LEU
1	A	613	HIS
1	A	617	ARG
1	A	631	LEU
1	A	633	LYS
1	A	634	LEU
1	A	636	THR
1	A	638	THR
1	A	640	LEU
1	A	641	GLU
1	A	645	VAL
1	A	646	VAL
1	A	650	ARG
1	A	655	LEU
1	A	743	ASP
1	A	744	ILE
1	A	751	LYS
1	A	752	LEU
1	A	761	ASN
1	A	762	VAL
1	A	768	LYS
1	A	774	MET
1	A	779	LEU
1	A	808	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	813	VAL
1	A	816	LEU
1	A	818	ARG
1	A	821	LEU
1	A	841	LEU
1	A	844	VAL
1	A	850	ILE
1	A	851	THR
1	A	874	LEU
1	A	914	THR
1	A	921	LEU
1	A	941	ILE
1	A	970	ASN
1	A	973	LEU
1	A	977	GLU
1	A	989	THR
1	A	1026	ARG
1	A	1027	LYS
1	A	1038	TRP
1	A	1043	VAL
1	A	1047	ARG
1	A	1057	MET
1	A	1060	LYS
1	A	1069	ILE
1	A	1074	VAL
1	A	1079	ILE
1	A	1081	ARG
1	A	1090	GLU
1	A	1091	GLU
1	A	1099	TRP
1	A	1118	TRP
1	A	1120	PHE
1	A	1129	PHE
1	A	1130	CYS
1	A	1133	ILE
1	A	1140	LEU
1	A	1141	VAL
1	A	1151	LEU
1	A	1191	LYS
1	A	1197	CYS
1	A	1198	LYS
1	A	1202	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1210	TYR
1	A	1218	LEU
2	B	69	LEU
2	B	83	LYS
2	B	186	LEU
2	B	218	VAL
2	B	231	ILE
2	B	240	VAL
2	B	263	TRP
2	B	332	VAL
2	B	338	VAL
2	B	364	LYS
2	B	365	LYS
2	B	368	HIS
2	B	372	LEU
2	B	394	GLU
2	B	396	ARG
2	B	413	VAL
2	B	428	LEU
2	B	441	VAL
2	B	444	THR
2	B	453	ILE
2	B	460	THR
2	B	461	THR
2	B	467	HIS
2	C	83	LYS
2	C	86	LEU
2	C	91	LEU
2	C	115	TRP
2	C	122	ARG
2	C	186	LEU
2	C	197	LEU
2	C	201	ASN
2	C	204	LEU
2	C	218	VAL
2	C	243	THR
2	C	251	TRP
2	C	256	LEU
2	C	262	TRP
2	C	281	GLU
2	C	282	GLU
2	C	293	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	295	TRP
2	C	300	ILE
2	C	331	VAL
2	C	371	VAL
2	C	402	LEU
2	C	413	VAL
2	C	419	GLU
2	C	453	ILE
2	C	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	159	GLN
1	A	298	HIS
1	A	354	ASN
1	A	388	ASN
1	A	497	GLN
1	A	754	HIS
1	A	828	HIS
1	A	906	HIS
1	A	971	HIS
1	A	975	GLN
2	C	124	GLN
2	C	210	GLN
2	C	258	HIS
2	C	292	ASN
2	C	313	HIS
2	C	409	ASN
2	C	427	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DOC	P	24	4,3	16,19,20	0.39	0	20,26,29	0.46	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DOC	P	24	4,3	-	0/7/18/19	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	DCT	A	4003	5	27,28,28	1.62	7 (25%)	37,43,43	1.17	3 (8%)

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	DCT	A	4003	5	-	2/22/31/31	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4003	DCT	C2-N1	-3.67	1.32	1.40
6	A	4003	DCT	C4-N4	3.59	1.42	1.33
6	A	4003	DCT	C1'-N1	-3.10	1.40	1.48
6	A	4003	DCT	C6-C5	2.55	1.41	1.35
6	A	4003	DCT	PB-O1B	2.31	1.58	1.50
6	A	4003	DCT	C3'-C2'	-2.24	1.47	1.54
6	A	4003	DCT	C2-N3	-2.18	1.32	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4003	DCT	C3'-C2'-C1'	3.35	106.73	102.87
6	A	4003	DCT	O2-C2-N3	-2.34	118.64	122.33
6	A	4003	DCT	N1-C2-N3	2.03	122.33	118.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

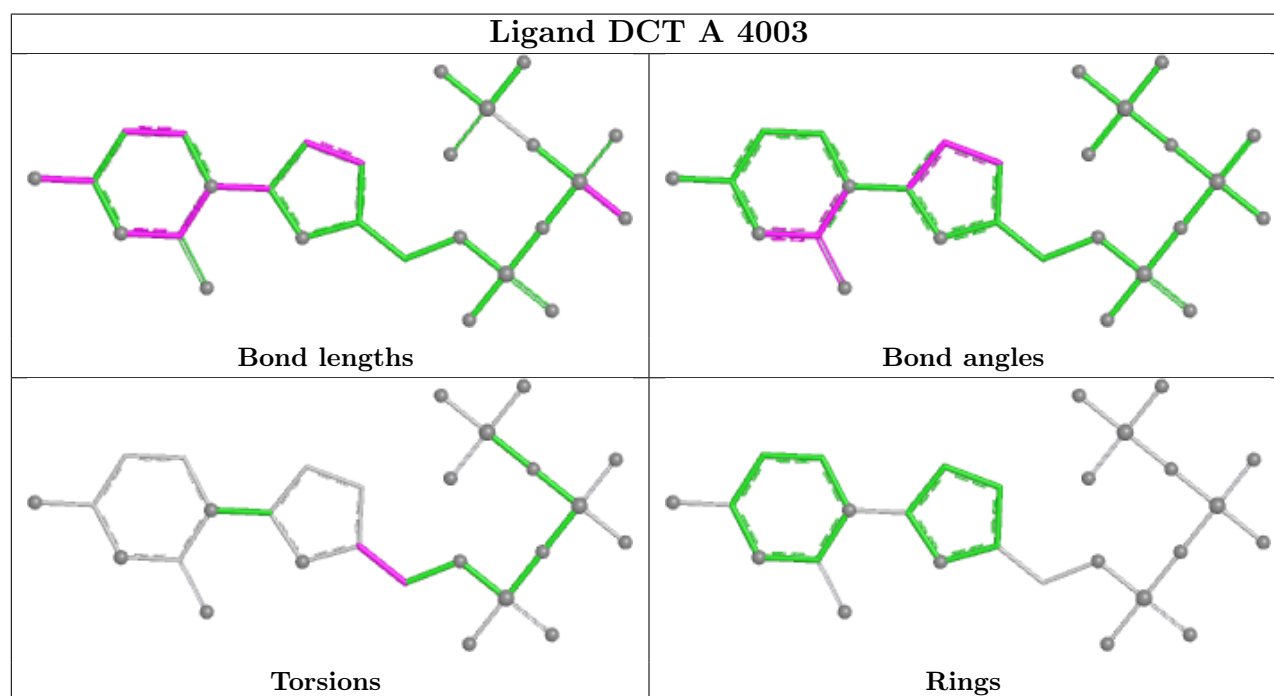
Mol	Chain	Res	Type	Atoms
6	A	4003	DCT	O4'-C4'-C5'-O5'
6	A	4003	DCT	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4003	DCT	2	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	983/1222 (80%)	0.62	81 (8%)	17	13	35, 71, 86, 91	0
2	B	363/472 (76%)	0.47	24 (6%)	24	16	46, 67, 83, 90	0
2	C	357/472 (75%)	0.33	13 (3%)	46	31	42, 70, 83, 90	0
3	T	25/27 (92%)	0.63	2 (8%)	18	14	74, 80, 92, 102	0
4	P	21/24 (87%)	0.65	0	100	100	71, 85, 99, 104	0
All	All	1749/2217 (78%)	0.53	120 (6%)	23	16	35, 70, 86, 104	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	759	SER	6.3
2	C	121	PHE	6.1
1	A	623	LEU	5.2
1	A	738	PRO	5.2
1	A	760	CYS	4.8
1	A	803	ASN	4.7
1	A	1127	GLY	4.6
1	A	1131	ILE	4.6
1	A	850	ILE	4.1
1	A	595	GLN	4.1
2	B	485	VAL	4.0
2	B	81	GLY	3.9
1	A	1082	ALA	3.8
1	A	912	GLY	3.7
1	A	610	PHE	3.7
2	B	304	TRP	3.7
1	A	1072	THR	3.6
2	C	355	GLN	3.6
2	B	388	GLY	3.6
1	A	507	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	642	SER	3.6
1	A	110	HIS	3.5
2	C	203	ARG	3.3
2	B	260	LEU	3.2
1	A	604	ALA	3.2
2	B	132	HIS	3.2
1	A	1219	ASP	3.2
2	B	393	LEU	3.2
2	B	243	THR	3.2
1	A	115	GLN	3.2
1	A	611	PRO	3.1
1	A	530	LEU	3.1
1	A	846	THR	3.1
2	B	82	SER	3.0
1	A	1025	LEU	3.0
1	A	227	ARG	3.0
1	A	622	TYR	3.0
1	A	1182	ALA	3.0
1	A	832	ASP	3.0
1	A	239	LEU	3.0
2	C	89	ASP	2.9
1	A	403	THR	2.9
1	A	572	TRP	2.8
1	A	915	ALA	2.8
1	A	1096	ARG	2.8
1	A	276	ALA	2.8
1	A	105	GLU	2.7
2	C	120	VAL	2.7
1	A	873	GLU	2.7
1	A	762	VAL	2.7
1	A	601	LYS	2.6
1	A	459	MET	2.6
1	A	962	ALA	2.6
1	A	429	GLU	2.6
2	C	68	ALA	2.6
1	A	1193	VAL	2.6
1	A	1213	PRO	2.5
2	C	316	PRO	2.5
1	A	764	SER	2.5
1	A	397	ALA	2.5
2	B	334	CYS	2.5
3	T	25	DT	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	1049	TRP	2.5
1	A	1199	THR	2.5
1	A	1057	MET	2.5
1	A	1055	SER	2.4
1	A	116	PRO	2.4
3	T	26	DT	2.4
1	A	414	PHE	2.4
2	C	264	ARG	2.4
2	B	367	LEU	2.4
1	A	563	PRO	2.4
2	C	420	THR	2.4
1	A	1075	LEU	2.4
1	A	619	GLY	2.3
2	B	273	PHE	2.3
1	A	620	TRP	2.3
1	A	957	ALA	2.3
1	A	1045	ALA	2.3
1	A	1221	TYR	2.3
2	B	185	LEU	2.3
1	A	598	VAL	2.3
1	A	635	PRO	2.3
2	B	468	ILE	2.3
2	C	81	GLY	2.3
1	A	766	PHE	2.3
2	B	390	GLY	2.2
1	A	605	LEU	2.2
2	B	97	PRO	2.2
1	A	277	HIS	2.2
1	A	363	TYR	2.2
1	A	1103	SER	2.2
1	A	1202	ASN	2.2
1	A	1185	ILE	2.2
1	A	508	ALA	2.2
1	A	877	MET	2.2
2	B	370	LYS	2.2
1	A	1134	HIS	2.2
2	C	228	VAL	2.1
1	A	986	TYR	2.1
2	B	79	LEU	2.1
1	A	634	LEU	2.1
1	A	841	LEU	2.1
1	A	94	MET	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	387	VAL	2.1
2	B	263	TRP	2.1
1	A	228	LEU	2.1
2	B	211	ILE	2.1
2	B	179	GLY	2.1
2	C	118	VAL	2.1
1	A	852	ARG	2.1
1	A	778	THR	2.1
2	B	318	ASN	2.0
2	C	442	LEU	2.0
1	A	1126	ASP	2.0
2	B	71	GLU	2.0
1	A	245	ILE	2.0
1	A	296	SER	2.0
1	A	120	LEU	2.0
1	A	612	LEU	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
4	DOC	P	24	18/19	0.92	0.12	51,77,117,118	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.

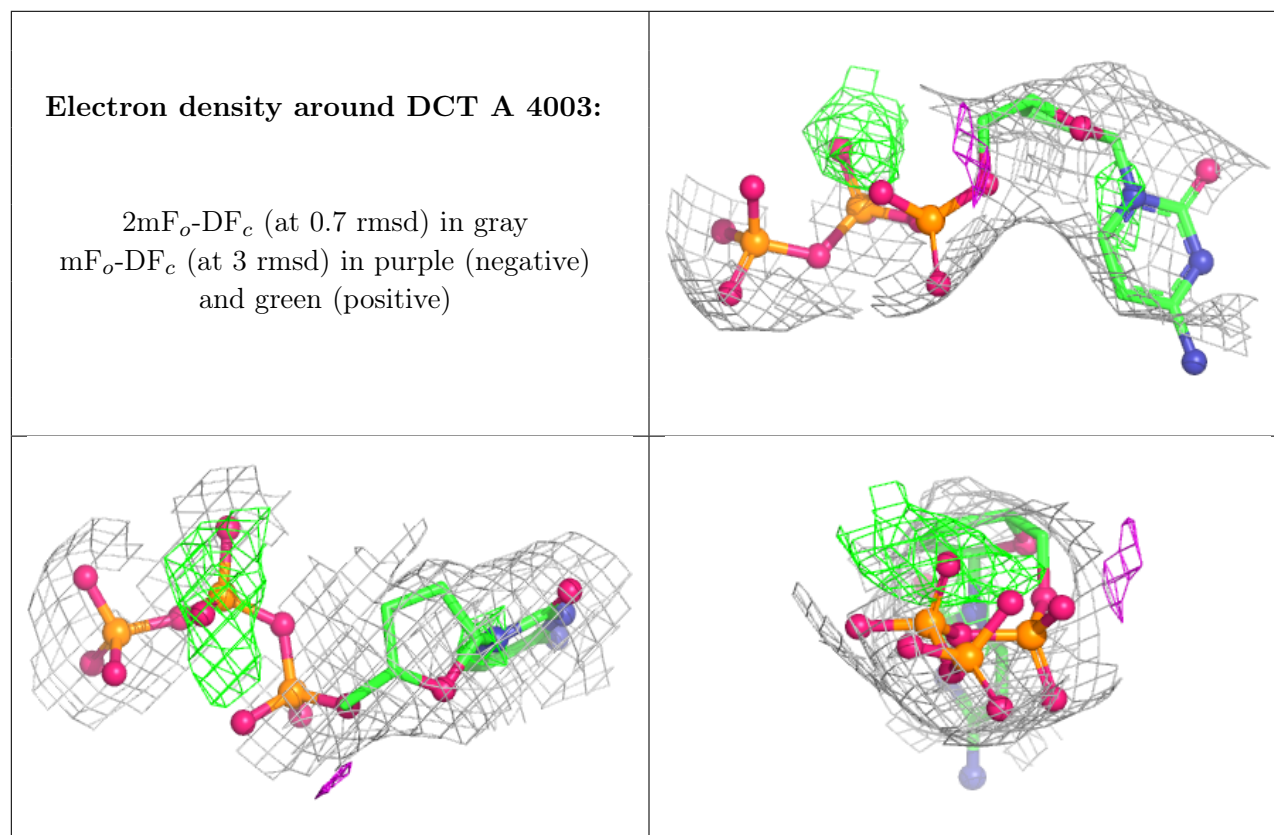
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	MG	A	4001	1/1	0.84	0.17	73,73,73,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	DCT	A	4003	27/27	0.90	0.13	68,81,115,118	0
5	MG	A	4002	1/1	0.98	0.04	35,35,35,35	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.