Full wwPDB X-ray Structure Validation Report ⓘ

Feb 25, 2024 – 02:38 AM EST

PDB ID	:	4ZTZ
Title	:	Structural basis for processivity and antiviral drug toxicity in human mitochondrial DNA replicase
Authors	:	Szymanski, M.R.; Yin, Y.W.
Deposited on	:	2015-05-15
Resolution	:	3.44 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:

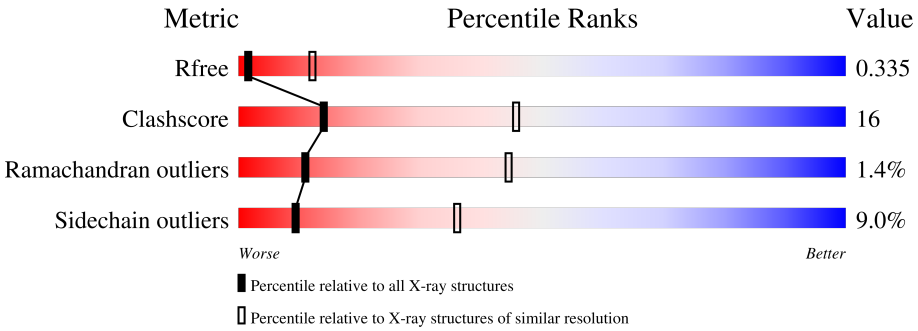
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.44 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)

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

Mol	Chain	Length	Quality of chain
1	A	1222	53% 23% . 20%
2	B	472	58% 17% . 23%
2	C	472	55% 17% . 24%
3	T	27	52% 41% 7%
4	P	24	54% 38% 8%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14651 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
			7823	4983	1371	1419	50			

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	conflict	UNP P54098
A	200	ALA	GLU	conflict	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	358	Total	C	N	O	S	0	0	0
			2893	1857	509	511	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			

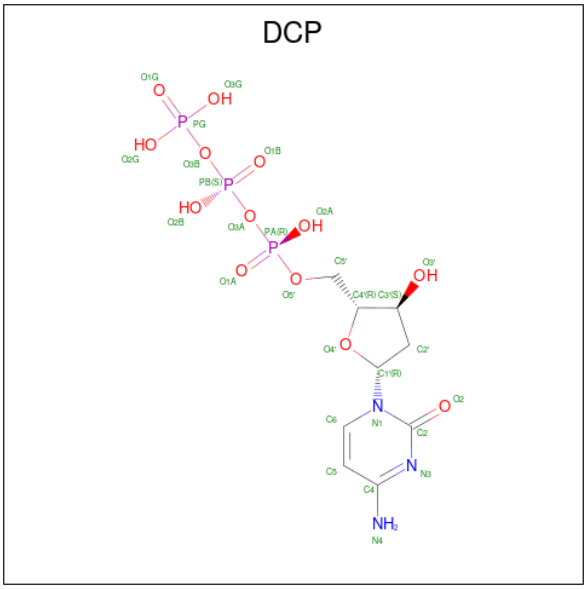
- Molecule 4 is a DNA chain called DNA (5'-D(P*AP*AP*GP*AP*CP*GP*AP*GP*GP*GP*CP*CP*AP*GP*TP*GP*CP*CP*GP*TP*AP*C)-3').

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 (three-letter code: MG) (formula: Mg).

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

- Molecule 6 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: $C_9H_{16}N_3O_{13}P_3$).



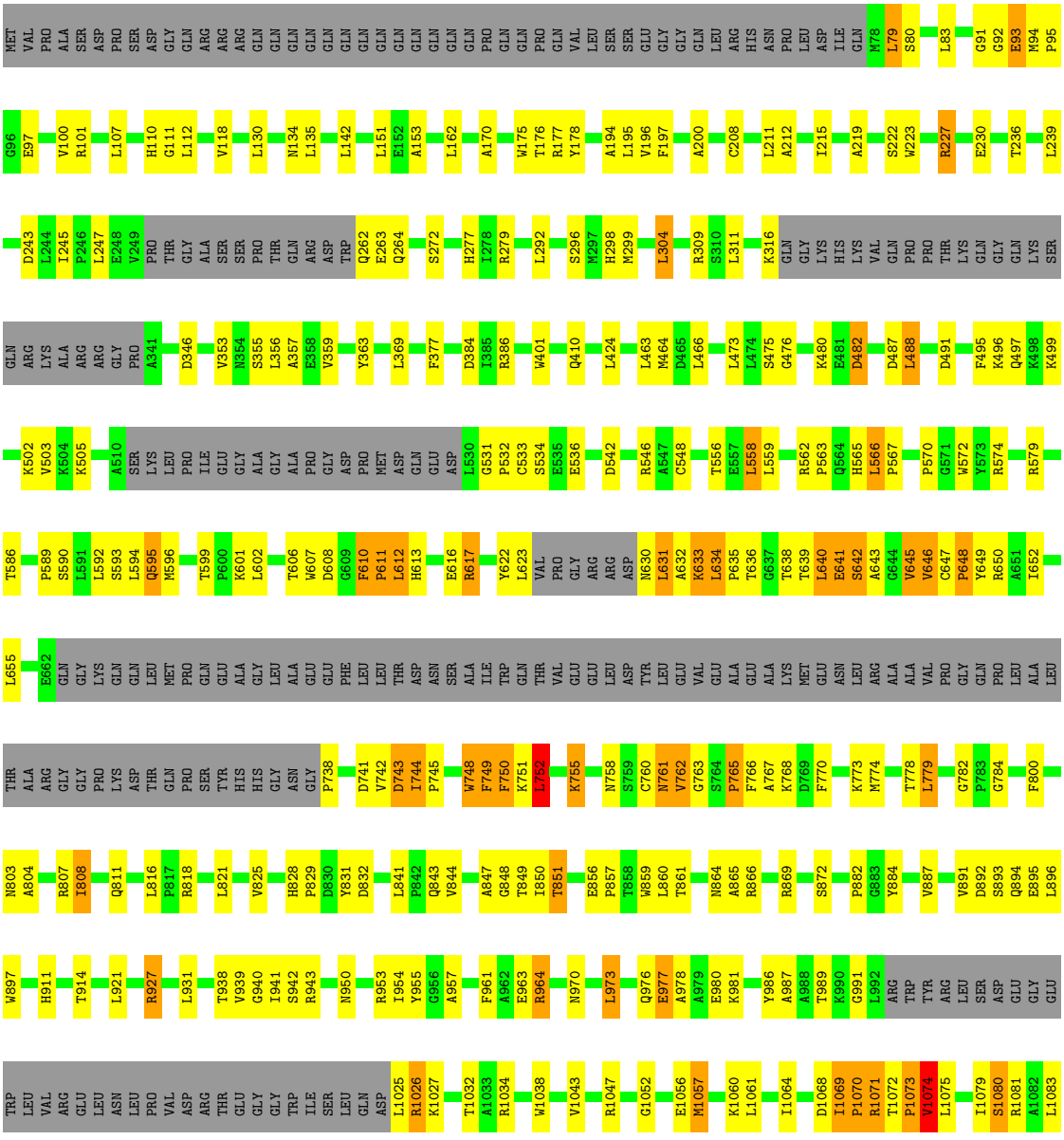
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			28	9	3	13	3		

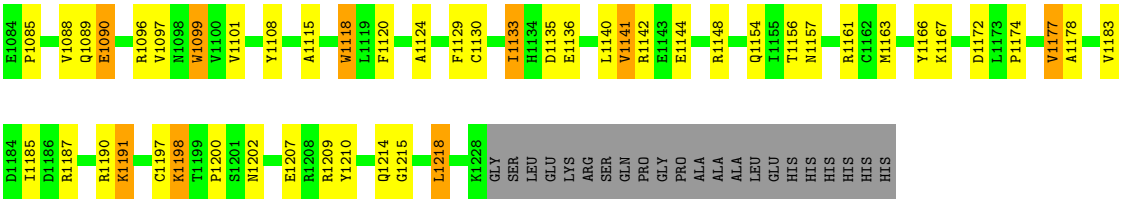
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 subunit gamma-1

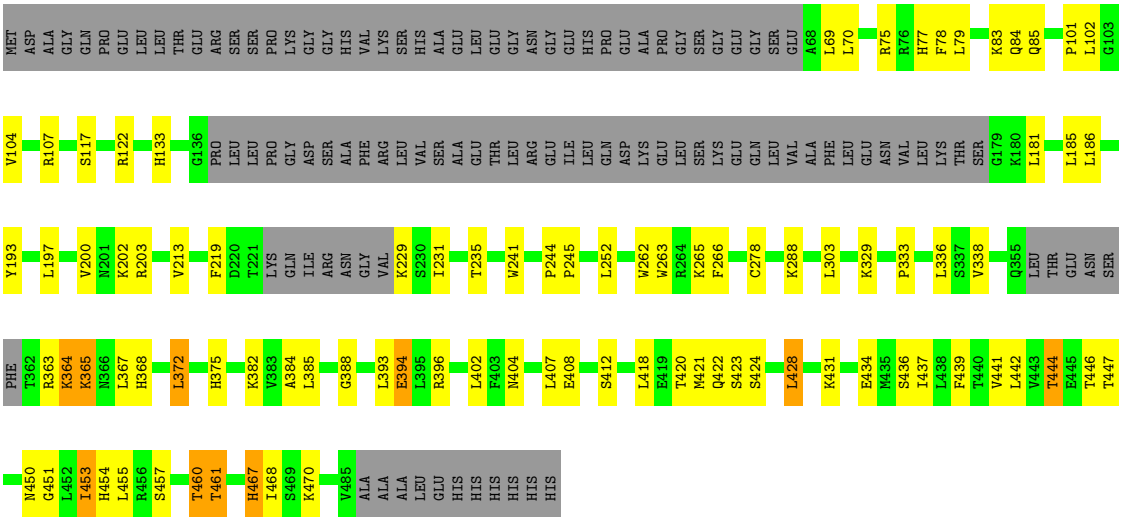
Chain A:





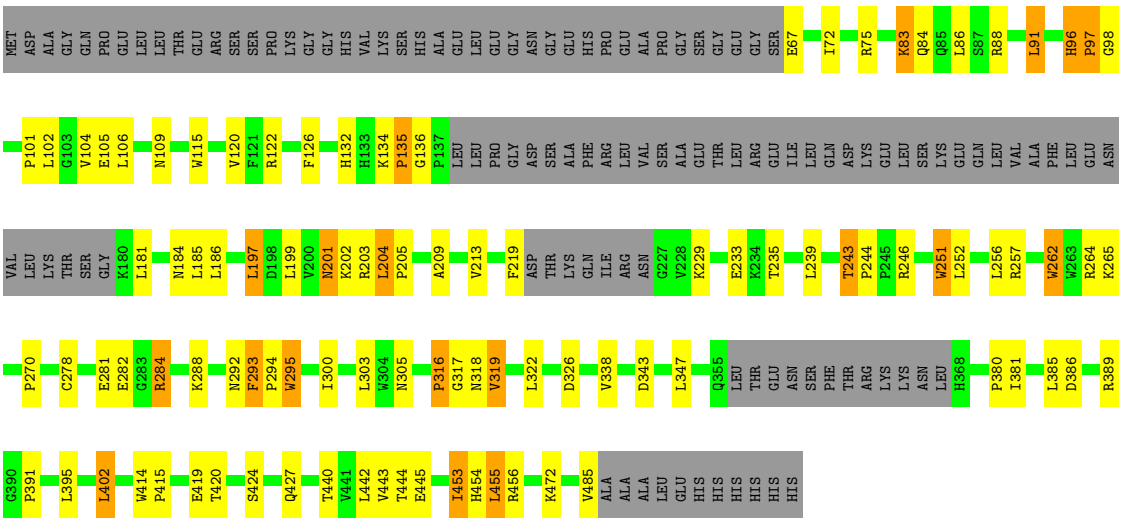
• Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

Chain B:



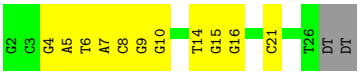
• Molecule 2: DNA polymerase subunit gamma-2, mitochondrial

Chain C:



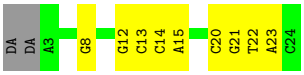
• Molecule 3: DNA (25-MER)

Chain T:



• 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')

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	217.60Å 217.60Å 165.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.50 – 3.44 49.25 – 3.45	Depositor EDS
% Data completeness (in resolution range)	91.6 (45.50-3.44) 95.2 (49.25-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.280 , 0.320 0.350 , 0.335	Depositor DCC
R_{free} test set	2000 reflections (3.97%)	wwPDB-VP
Wilson B-factor (Å^2)	140.7	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 20.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	14651	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 2.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	1/8025 (0.0%)	0.48	6/10886 (0.1%)
2	B	0.21	0/3015	0.39	0/4074
2	C	0.23	0/2966	0.45	2/4009 (0.0%)
3	T	0.47	0/567	0.88	0/872
4	P	0.49	0/492	0.77	0/758
All	All	0.27	1/15065 (0.0%)	0.50	8/20599 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	611	PRO	N-CD	-10.82	1.32	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	611	PRO	N-CA-CB	-11.49	89.52	103.30
2	C	135	PRO	CA-N-CD	-8.60	99.46	111.50
2	C	96	HIS	C-N-CD	-8.37	102.18	120.60
1	A	611	PRO	N-CD-CG	-6.82	92.97	103.20
1	A	752	LEU	C-N-CD	-6.27	106.81	120.60
1	A	611	PRO	CA-N-CD	6.08	120.21	111.70
1	A	610	PHE	N-CA-C	5.65	126.25	111.00
1	A	482	ASP	CB-CG-OD2	5.21	122.99	118.30

There are no chirality outliers.

There are no planarity outliers.

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	7823	0	7729	293	0
2	B	2942	0	2939	58	0
2	C	2893	0	2880	97	0
3	T	508	0	282	15	0
4	P	455	0	245	8	0
5	A	2	0	0	0	0
6	A	28	0	12	4	0
All	All	14651	0	14087	452	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (452) 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:610:PHE:CE1	1:A:652:ILE:HD13	1.26	1.70
1:A:610:PHE:CD1	1:A:611:PRO:HG3	1.19	1.67
1:A:610:PHE:CE1	1:A:611:PRO:HG3	1.12	1.64
1:A:610:PHE:CG	1:A:611:PRO:HD3	1.29	1.59
1:A:610:PHE:CD1	1:A:611:PRO:CG	1.80	1.58
1:A:610:PHE:CE1	1:A:611:PRO:CG	1.83	1.53
1:A:634:LEU:CD2	1:A:635:PRO:HD2	1.37	1.50
1:A:634:LEU:HD23	1:A:635:PRO:CD	1.39	1.49
1:A:610:PHE:CD1	1:A:611:PRO:CD	1.98	1.45
1:A:610:PHE:CE1	1:A:652:ILE:CD1	2.14	1.30
1:A:631:LEU:C	1:A:633:LYS:CE	1.95	1.27
1:A:610:PHE:CD1	1:A:611:PRO:HD3	1.66	1.27
1:A:649:TYR:CD2	1:A:750:PHE:CE2	2.25	1.25
1:A:631:LEU:C	1:A:633:LYS:HE2	1.38	1.25
1:A:640:LEU:C	1:A:640:LEU:HD22	1.61	1.20
1:A:632:ALA:C	1:A:633:LYS:HD3	1.62	1.19
1:A:640:LEU:HD22	1:A:640:LEU:O	1.41	1.18
1:A:610:PHE:CG	1:A:611:PRO:CD	2.17	1.16
1:A:610:PHE:CZ	1:A:748:TRP:HB3	1.80	1.15
1:A:610:PHE:CD1	1:A:652:ILE:HD13	1.81	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:LEU:O	1:A:633:LYS:HE2	1.44	1.12
2:C:135:PRO:HD2	2:C:136:GLY:H	1.10	1.11
1:A:649:TYR:HB3	1:A:750:PHE:CZ	1.84	1.11
1:A:610:PHE:CZ	1:A:652:ILE:HD13	1.85	1.10
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:649:TYR:CG	1:A:750:PHE:CE2	2.47	1.03
1:A:610:PHE:CD1	1:A:652:ILE:CD1	2.40	1.01
1:A:641:GLU:HG3	1:A:642:SER:H	1.09	1.01
1:A:610:PHE:CE1	1:A:611:PRO:HG2	1.96	1.00
2:C:134:LYS:HD2	2:C:135:PRO:CD	1.92	1.00
2:C:102:LEU:O	2:C:105:GLU:CD	2.00	0.99
2:C:134:LYS:HD2	2:C:135:PRO:HD3	1.00	0.99
1:A:610:PHE:CD2	1:A:611:PRO:HD3	1.98	0.97
1:A:632:ALA:O	1:A:633:LYS:HD3	1.66	0.95
1:A:610:PHE:HE1	1:A:611:PRO:HG3	1.21	0.95
1:A:610:PHE:CD1	1:A:652:ILE:CG1	2.52	0.93
2:C:419:GLU:H	2:C:420:THR:HA	1.32	0.92
1:A:610:PHE:CE2	1:A:748:TRP:HB3	2.04	0.92
2:C:101:PRO:O	2:C:105:GLU:HG3	1.69	0.92
1:A:640:LEU:C	1:A:640:LEU:CD2	2.36	0.92
1:A:649:TYR:CB	1:A:750:PHE:CZ	2.53	0.90
1:A:649:TYR:CD2	1:A:750:PHE:HE2	1.84	0.90
1:A:610:PHE:CE2	1:A:748:TRP:CB	2.55	0.89
2:C:135:PRO:HD2	2:C:136:GLY:N	1.87	0.89
1:A:473:LEU:HD22	1:A:482:ASP:OD2	1.73	0.88
1:A:738:PRO:O	1:A:742:VAL:HG21	1.73	0.88
2:C:134:LYS:NZ	2:C:135:PRO:HD2	1.90	0.87
1:A:610:PHE:CD1	1:A:652:ILE:HG12	2.09	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	0.86
1:A:649:TYR:CD2	1:A:750:PHE:CD2	2.64	0.85
1:A:610:PHE:HD1	1:A:611:PRO:HG3	1.31	0.85
1:A:649:TYR:CG	1:A:750:PHE:CD2	2.64	0.85
1:A:738:PRO:O	1:A:742:VAL:CG2	2.23	0.85
1:A:632:ALA:C	1:A:633:LYS:CD	2.45	0.84
2:C:67:GLU:HG3	2:C:88:ARG:NH2	1.94	0.83
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
1:A:649:TYR:CB	1:A:750:PHE:CE2	2.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:PHE:HD1	1:A:611:PRO:CG	1.85	0.81
2:C:134:LYS:CD	2:C:135:PRO:CD	2.54	0.80
1:A:610:PHE:CZ	1:A:748:TRP:CB	2.65	0.79
1:A:641:GLU:CG	1:A:642:SER:N	2.44	0.78
2:C:101:PRO:O	2:C:105:GLU:CG	2.31	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
1:A:649:TYR:HB3	1:A:750:PHE:CE2	2.19	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:744:ILE:HG23	1:A:745:PRO:HD3	1.68	0.75
2:C:105:GLU:CD	2:C:106:LEU:H	1.90	0.75
2:C:134:LYS:HZ2	2:C:135:PRO:HD2	1.52	0.74
1:A:623:LEU:HA	1:A:760:CYS:SG	2.28	0.73
2:C:102:LEU:C	2:C:105:GLU:CD	2.46	0.73
1:A:473:LEU:CD2	1:A:482:ASP:OD2	2.35	0.73
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:760:CYS:SG	1:A:762:VAL:CG1	2.79	0.71
1:A:610:PHE:CD1	1:A:611:PRO:N	2.58	0.71
1:A:633:LYS:HD3	1:A:633:LYS:N	1.95	0.71
1:A:631:LEU:N	1:A:631:LEU:HD23	2.04	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:630:ASN:C	1:A:631:LEU:HD23	2.11	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:610:PHE:CE2	1:A:748:TRP:HB2	2.26	0.69
1:A:649:TYR:HD2	1:A:750:PHE:HE2	1.39	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:101:PRO:O	2:C:105:GLU:CD	2.32	0.68
1:A:760:CYS:SG	1:A:762:VAL:HG13	2.35	0.67
1:A:850:ILE:HG22	3:T:6:DT:H4'	1.75	0.67
1:A:463:LEU:HD21	1:A:594:LEU:HD23	1.77	0.67
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:884:TYR:HA	1:A:1142:ARG:HA	1.78	0.64
2:C:201:ASN:CB	2:C:203:ARG:NH1	2.61	0.64
2:C:213:VAL:HG22	2:C:235:THR:HG22	1.77	0.64
2:C:134:LYS:HZ3	2:C:135:PRO:CD	2.11	0.64
2:B:442:LEU:HB3	2:B:454:HIS:HB2	1.80	0.63
1:A:642:SER:OG	1:A:643:ALA:HA	1.98	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
2:C:67:GLU:HG3	2:C:88:ARG:HH22	1.64	0.62
1:A:632:ALA:N	1:A:633:LYS:NZ	2.42	0.62
1:A:642:SER:OG	1:A:643:ALA:CA	2.47	0.62
1:A:866:ARG:HH21	1:A:869:ARG:HD2	1.64	0.62
1:A:921:LEU:HD22	1:A:1174:PRO:HG2	1.82	0.62
1:A:623:LEU:CA	1:A:760:CYS:SG	2.88	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
2:C:265:LYS:CD	2:C:485:VAL:HG22	2.29	0.62
1:A:649:TYR:CG	1:A:649:TYR:O	2.53	0.61
1:A:953:ARG:HA	1:A:957:ALA:HB2	1.82	0.61
2:C:197:LEU:HD12	2:C:202:LYS:HG2	1.82	0.61
1:A:760:CYS:SG	1:A:762:VAL:HG12	2.39	0.61
2:B:382:LYS:H	2:B:412:SER:HB2	1.65	0.61
2:C:292:ASN:HD21	2:C:294:PRO:HB3	1.65	0.61
2:C:201:ASN:HB3	2:C:203:ARG:NH1	2.16	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:102:LEU:O	2:C:105:GLU:CG	2.50	0.60
1:A:79:LEU:H	1:A:83:LEU:HG	1.66	0.59
2:C:83:LYS:HG2	2:C:84:GLN:HG2	1.84	0.59
1:A:938:THR:N	1:A:939:VAL:HA	2.16	0.59
1:A:623:LEU:C	1:A:760:CYS:SG	2.81	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
2:C:105:GLU:CD	2:C:106:LEU:N	2.54	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:135:PRO:CD	2:C:136:GLY:N	2.55	0.59
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
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
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
1:A:634:LEU:HD23	1:A:635:PRO:HD2	0.63	0.58
1:A:610:PHE:HE1	1:A:611:PRO:CG	1.90	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:299:MET:HE3	1:A:848:GLY:HA2	1.86	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
1:A:610:PHE:CE1	1:A:611:PRO:CD	2.59	0.57
2:C:246:ARG:NH2	2:C:326:ASP:OD2	2.38	0.57
1:A:196:VAL:HG22	1:A:215:ILE:HG12	1.87	0.56
1:A:230:GLU:OE2	1:A:386:ARG:NH1	2.38	0.56
1:A:262:GLN:HB2	1:A:263:GLU:HG2	1.87	0.56
2:B:444:THR:HG23	2:B:446:THR:H	1.69	0.56
1:A:825:VAL:HG13	1:A:882:PRO:HG2	1.86	0.56
1:A:200:ALA:HB3	1:A:211:LEU:HB2	1.88	0.56
1:A:1073:PRO:HA	1:A:1074:VAL:HG13	1.88	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
1:A:649:TYR:CD2	1:A:649:TYR:O	2.59	0.56
2:B:252:LEU:HD13	2:B:336:LEU:HD11	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:201:ASN:HB3	2:C:203:ARG:HG3	1.88	0.55
2:B:446:THR:O	2:B:450:ASN:ND2	2.40	0.55
2:C:134:LYS:CG	2:C:135:PRO:CD	2.84	0.55
2:C:235:THR:OG1	2:C:343:ASP:OD1	2.22	0.55
1:A:107:LEU:O	1:A:112:LEU:N	2.35	0.54
1:A:579:ARG:NH1	4:P:12:DG:OP1	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:457:SER:OG	2:B:460:THR:O	2.25	0.54
2:C:201:ASN:HB2	2:C:203:ARG:NH1	2.22	0.54
2:B:428:LEU:HD13	2:B:428:LEU:H	1.72	0.54
1:A:647:CYS:SG	1:A:648:PRO:CD	2.96	0.54
2:C:201:ASN:HB3	2:C:203:ARG:HH11	1.72	0.54
1:A:1124:ALA:O	1:A:1148:ARG:NH2	2.40	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	1.91	0.53
2:C:444:THR:OG1	2:C:445:GLU:N	2.36	0.53
2:C:319:VAL:HA	2:C:322:LEU:HD13	1.89	0.53
1:A:566:LEU:HD13	1:A:566:LEU:H	1.73	0.53
2:B:262:TRP:HA	2:B:265:LYS:HE2	1.91	0.53
1:A:353:VAL:HG13	1:A:355:SER:H	1.74	0.53
1:A:466:LEU:HB3	1:A:602:LEU:HD21	1.90	0.53
1:A:649:TYR:CE1	1:A:749:PHE:O	2.62	0.53
1:A:864:ASN:O	1:A:872:SER:OG	2.25	0.53
1:A:610:PHE:CG	1:A:652:ILE:CG1	2.83	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: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:639:THR:HG22	1:A:640:LEU:N	2.25	0.52
2:B:185:LEU:H	2:B:185:LEU:HD23	1.74	0.52
1:A:642:SER:OG	1:A:643:ALA:HB2	2.09	0.52
1:A:647:CYS:SG	1:A:648:PRO:N	2.83	0.52
1:A:631:LEU:N	1:A:631:LEU:CD2	2.72	0.51
1:A:894:GLN:HG3	1:A:895:GLU:H	1.75	0.51
1:A:895:GLU:HB2	6:A:4003:DCP:O3'	2.10	0.51
1:A:212:ALA:HB3	1:A:223:TRP:HB3	1.92	0.51
2:B:407:LEU:HD13	2:C:120:VAL:HG12	1.92	0.51
1:A:743:ASP:OD1	1:A:743:ASP:N	2.35	0.51
1:A:384:ASP:OD1	1:A:384:ASP:N	2.40	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:634:LEU:CG	1:A:635:PRO:HD2	2.31	0.51
1:A:272:SER:HB3	1:A:843:GLN:HA	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:THR:OG1	1:A:222:SER:OG	2.26	0.51
1:A:162:LEU:HG	1:A:401:TRP:CZ3	2.46	0.50
2:B:278:CYS:SG	2:B:288:LYS:NZ	2.84	0.50
1:A:175:TRP:CD2	1:A:223:TRP:HB2	2.45	0.50
1:A:211:LEU:HD12	1:A:377:PHE:HZ	1.76	0.50
1:A:861:THR:HG21	3:T:8:DC:H1'	1.92	0.50
1:A:1069:ILE:O	1:A:1071:ARG:N	2.44	0.50
2:C:104:VAL:N	2:C:105:GLU:CD	2.64	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
3:T:14:DT:H2"	3:T:15:DG:C8	2.47	0.50
1:A:639:THR:HG22	1:A:640:LEU:H	1.77	0.50
1:A:641:GLU:OE1	1:A:642:SER:O	2.30	0.50
2:C:264:ARG:HG3	2:C:270:PRO:HB3	1.92	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
1:A:610:PHE:CG	1:A:652:ILE:HG12	2.44	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
2:C:96:HIS:HB3	2:C:97:PRO:C	2.32	0.49
3:T:4:DG:C2	3:T:5:DA:C4	3.00	0.49
1:A:803:ASN:HA	3:T:10:DG:H4'	1.92	0.49
2:B:418:LEU:HD22	2:C:204:LEU:HD12	1.94	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
2:C:134:LYS:HZ3	2:C:135:PRO:HD2	1.70	0.49
1:A:546:ARG:NH2	2:B:408:GLU:OE2	2.45	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
4:P:14:DC:H2'	4:P:15:DA:C8	2.48	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: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
1:A:562:ARG:HD2	1:A:563:PRO:HD2	1.95	0.48
1:A:495:PHE:HB3	1:A:496:LYS:HB2	1.94	0.48
1:A:616:GLU:HB2	1:A:617:ARG:HD3	1.96	0.48
2:B:388:GLY:HA3	2:B:442:LEU:HD11	1.94	0.48
3:T:9:DG:H2'	3:T:10:DG:C8	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:VAL:HA	2:B:235:THR:HA	1.96	0.48
2:C:424:SER:HB3	2:C:427:GLN:HG2	1.95	0.48
3:T:16:DG:H1	4:P:13:DC:H42	1.61	0.48
3:T:21:DC:H42	4:P:8:DG:H1	1.61	0.48
1:A:1187:ARG:HH11	1:A:1209:ARG:HH12	1.61	0.48
1:A:631:LEU:O	1:A:633:LYS:HE3	2.10	0.48
1:A:761:ASN:OD1	1:A:761:ASN:N	2.47	0.48
2:B:219:PHE:HA	2:B:229:LYS:N	2.29	0.48
1:A:357:ALA:HA	1:A:369:LEU:HD21	1.96	0.48
1:A:897:TRP:CD1	1:A:1177:VAL:HG21	2.48	0.48
1:A:91:GLY:HA2	1:A:92:GLY:HA3	1.58	0.47
1:A:1200:PRO:O	1:A:1202:ASN:N	2.43	0.47
2:B:404:ASN:HA	2:B:407:LEU:HG	1.95	0.47
1:A:645:VAL:O	1:A:645:VAL:CG1	2.60	0.47
1:A:1214:GLN:HA	1:A:1215:GLY:HA3	1.58	0.47
2:C:201:ASN:CB	2:C:203:ARG:HH11	2.27	0.47
1:A:1068:ASP:OD2	1:A:1068:ASP:N	2.46	0.47
2:B:428:LEU:HA	2:B:431:LYS:HB3	1.95	0.47
2:C:293:PHE:HB3	2:C:295:TRP:H	1.79	0.47
1:A:939:VAL:HA	1:A:940:GLY:HA3	1.71	0.47
1:A:135:LEU:HD23	1:A:135:LEU:H	1.80	0.47
1:A:491:ASP:HB2	1:A:574:ARG:HH12	1.80	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:480:LYS:HD3	1:A:646:VAL:HG11	1.97	0.47
1:A:649:TYR:HD2	1:A:750:PHE:CE2	2.08	0.47
1:A:304:LEU:HD13	1:A:309:ARG:HG2	1.96	0.47
1:A:612:LEU:HD12	1:A:612:LEU:HA	1.83	0.47
1:A:976:GLN:O	1:A:980:GLU:HG2	2.15	0.47
1:A:1069:ILE:CB	1:A:1070:PRO:HD2	2.45	0.47
2:C:303:LEU:HD22	2:C:338:VAL:HG22	1.97	0.47
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
2:C:265:LYS:HD2	2:C:485:VAL:HG22	1.97	0.46
1:A:642:SER:OG	1:A:643:ALA:CB	2.64	0.46
1:A:869:ARG:NH1	4:P:22:DT:OP1	2.48	0.46
1:A:1135:ASP:HB2	6:A:4003:DCP:H5'2	1.97	0.46
1:A:1163:MET:SD	1:A:1167:LYS:HE2	2.55	0.46
1:A:955:TYR:CE2	3:T:4:DG:N2	2.83	0.46
2:B:363:ARG:O	2:B:364:LYS:HG3	2.15	0.46
4:P:22:DT:H2'	4:P:23:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:O	1:A:219:ALA:HB1	2.16	0.46
2:C:91:LEU:HD12	2:C:347:LEU:HD21	1.97	0.46
2:B:402:LEU:HD13	2:B:468:ILE:HG23	1.98	0.46
2:C:67:GLU:N	2:C:88:ARG:HH21	2.13	0.46
1:A:640:LEU:HD22	1:A:641:GLU:N	2.24	0.46
1:A:942:SER:HA	1:A:943:ARG:HA	1.59	0.46
2:B:78:PHE:HD2	2:C:199:LEU:HD13	1.79	0.46
1:A:778:THR:HA	1:A:779:LEU:HA	1.60	0.46
1:A:272:SER:OG	1:A:844:VAL:O	2.34	0.46
1:A:634:LEU:CD2	1:A:635:PRO:CD	2.30	0.46
1:A:1060:LYS:O	1:A:1064:ILE:HG12	2.16	0.46
1:A:1079:ILE:HG12	1:A:1099:TRP:CZ3	2.51	0.46
1:A:298:HIS:HB2	1:A:410:GLN:HE22	1.79	0.45
1:A:1061:LEU:HB3	1:A:1097:VAL:HG13	1.98	0.45
2:B:133:HIS:ND1	2:C:233:GLU:OE2	2.48	0.45
1:A:599:THR:HA	1:A:602:LEU:HB3	1.99	0.45
1:A:562:ARG:HH11	1:A:563:PRO:HD2	1.81	0.45
2:B:193:TYR:OH	2:B:333:PRO:HG3	2.16	0.45
2:C:239:LEU:HB3	2:C:338:VAL:HB	1.98	0.45
1:A:741:ASP:HB3	1:A:745:PRO:HB2	1.98	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:C:72:ILE:HA	2:C:75:ARG:HG2	1.97	0.45
2:C:316:PRO:HA	2:C:317:GLY:HA2	1.48	0.45
2:C:105:GLU:O	2:C:109:ASN:ND2	2.47	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: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	0.45
2:B:181:LEU:HD21	2:C:181:LEU:HD21	1.99	0.45
1:A:586:THR:OG1	1:A:590:SER:OG	2.30	0.44
2:B:200:VAL:HG13	2:B:203:ARG:H	1.82	0.44
1:A:608:ASP:OD1	1:A:778:THR:OG1	2.26	0.44
1:A:991:GLY:HA2	1:A:1052:GLY:HA2	1.99	0.44
2:C:317:GLY:HA3	2:C:318:ASN:HA	1.61	0.44
1:A:556:THR:HA	1:A:559:LEU:HD13	1.99	0.44
1:A:649:TYR:HE1	1:A:749:PHE:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:421:MET:HA	2:B:422:GLN:HB3	2.00	0.44
1:A:593:SER:C	1:A:596:MET:H	2.21	0.44
1:A:239:LEU:HD13	1:A:239:LEU:HA	1.85	0.44
2:C:102:LEU:O	2:C:105:GLU:HG2	2.17	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
2:B:101:PRO:HB3	2:C:126:PHE:HB3	1.99	0.44
2:C:134:LYS:HZ2	2:C:136:GLY:H	1.66	0.44
1:A:646:VAL:CG2	1:A:647:CYS:N	2.79	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:973:LEU:HD22	1:A:976:GLN:H	1.83	0.44
2:B:372:LEU:HD13	2:B:436:SER:HB2	1.99	0.44
2:C:265:LYS:HD3	2:C:485:VAL:HG22	1.98	0.44
1:A:497:GLN:NE2	1:A:559:LEU:HB3	2.32	0.44
1:A:987:ALA:HB1	1:A:1056:GLU:HG2	2.00	0.44
2:B:365:LYS:HG2	2:B:367:LEU:H	1.83	0.44
4:P:22:DT:H2'	4:P:23:DA:H8	1.83	0.44
1:A:475:SER:HA	1:A:476:GLY:HA2	1.50	0.43
1:A:632:ALA:C	1:A:633:LYS:CE	2.87	0.43
1:A:1079:ILE:H	1:A:1079:ILE:HG13	1.70	0.43
2:B:79:LEU:HG	2:B:102:LEU:HB2	2.00	0.43
3:T:4:DG:N3	3:T:5:DA:C8	2.85	0.43
2:C:134:LYS:CE	2:C:135:PRO:HD3	2.47	0.43
2:B:365:LYS:H	2:B:365:LYS:HD2	1.83	0.43
2:B:447:THR:HG21	2:B:453:ILE:HA	2.00	0.43
1:A:856:GLU:N	1:A:860:LEU:HD12	2.33	0.43
1:A:963:GLU:HG3	1:A:981:LYS:NZ	2.33	0.43
1:A:1079:ILE:HG12	1:A:1099:TRP:CE3	2.53	0.43
1:A:1154:GLN:HG3	1:A:1218:LEU:HD21	2.00	0.43
1:A:299:MET:HG3	1:A:849:THR:HG23	2.01	0.43
1:A:1080:SER:OG	1:A:1083:LEU:HB2	2.19	0.43
3:T:6:DT:H2'	3:T:7:DA:O4'	2.18	0.43
6:A:4003:DCP:N3	3:T:4:DG:N1	2.58	0.43
2:B:197:LEU:HD23	2:B:197:LEU:HA	1.88	0.43
2:B:266:PHE:HA	2:B:375:HIS:CD2	2.53	0.43
2:C:292:ASN:ND2	2:C:294:PRO:HB3	2.32	0.43
2:C:209:ALA:HB2	2:C:239:LEU:HD13	1.99	0.43
1:A:298:HIS:CD2	1:A:363:TYR:HE1	2.36	0.43
1:A:950:ASN:O	1:A:954:ILE:HG13	2.18	0.43
2:C:67:GLU:HG3	2:C:88:ARG:HH21	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:GLU:OE1	1:A:859:TRP:N	2.36	0.43
1:A:1088:VAL:HG12	1:A:1090:GLU:HA	2.00	0.43
2:C:105:GLU:HG2	2:C:380:PRO:HB3	2.00	0.43
1:A:891:VAL:HG13	1:A:1161:ARG:HH12	1.83	0.42
1:A:865:ALA:HB2	1:A:1191:LYS:HZ2	1.84	0.42
2:B:303:LEU:HG	2:B:338:VAL:HB	2.01	0.42
1:A:536:GLU:HG3	2:C:257:ARG:HH12	1.84	0.42
1:A:567:PRO:HA	1:A:574:ARG:HE	1.84	0.42
1:A:892:ASP:HA	1:A:893:SER:HA	1.66	0.42
2:B:213:VAL:HG11	2:C:132:HIS:CE1	2.53	0.42
2:C:265:LYS:HD3	2:C:485:VAL:CG2	2.48	0.42
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.90	0.42
1:A:1108:TYR:CE1	1:A:1161:ARG:HD3	2.54	0.42
2:B:83:LYS:HG2	2:B:85:GLN:H	1.85	0.42
2:C:134:LYS:HZ3	2:C:135:PRO:CG	2.32	0.42
4:P:20:DC:H2"	4:P:21:DG:C8	2.54	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
1:A:807:ARG:HD3	3:T:9:DG:H4'	2.00	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:134:LYS:HZ3	2:C:135:PRO:HG2	1.85	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:586:THR:HG1	1:A:590:SER:HG	1.60	0.42
1:A:955:TYR:CD2	3:T:4:DG:N2	2.88	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
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
1:A:649:TYR:HB2	1:A:750:PHE:CE1	2.55	0.41
2:C:243:THR:HG1	2:C:251:TRP:HE3	1.66	0.41
2:C:293:PHE:N	2:C:294:PRO:HA	2.35	0.41
1:A:531:GLY:HA2	1:A:532:PRO:HD3	1.84	0.41
2:B:364:LYS:HB2	2:B:364:LYS:HE2	1.63	0.41
2:C:278:CYS:SG	2:C:288:LYS:NZ	2.92	0.41
1:A:505:LYS:HA	1:A:505:LYS:HD3	1.76	0.41
2:C:134:LYS:CE	2:C:135:PRO:CD	2.98	0.41
1:A:298:HIS:HB2	1:A:410:GLN:NE2	2.35	0.41
1:A:856:GLU:HA	1:A:857:PRO:HD3	1.88	0.41
2:B:384:ALA:HB2	2:B:437:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:TRP:HA	1:A:778:THR:HG23	2.01	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
1:A:953:ARG:HG3	1:A:957:ALA:HB2	2.02	0.41
2:C:472:LYS:HE2	2:C:472:LYS:HB3	1.91	0.41
1:A:110:HIS:HB3	1:A:111:GLY:HA2	2.01	0.41
1:A:606:THR:HG21	1:A:612:LEU:N	2.36	0.41
1:A:961:PHE:O	1:A:964:ARG:HD2	2.20	0.41
1:A:1198:LYS:HB3	1:A:1198:LYS:HE3	1.84	0.41
1:A:828:HIS:CG	1:A:829:PRO:HD2	2.55	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	0.41
1:A:356:LEU:HA	1:A:359:VAL:HG12	2.02	0.41
1:A:641:GLU:CG	1:A:642:SER:H	2.01	0.40
1:A:97:GLU:HA	1:A:100:VAL:HG22	2.03	0.40
1:A:1025:LEU:HB3	1:A:1026:ARG:H	1.68	0.40
2:C:385:LEU:HD22	2:C:402:LEU:HD13	2.03	0.40
2:C:284:ARG:CZ	2:C:284:ARG:HA	2.51	0.40
6:A:4003:DCP:N4	3:T:4:DG:O6	2.55	0.40
2:B:70:LEU:HD23	2:B:70:LEU:H	1.86	0.40
2:B:244:PRO:HA	2:B:245:PRO:HD3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	969/1222 (79%)	846 (87%)	106 (11%)	17 (2%)	8 39
2	B	355/472 (75%)	326 (92%)	27 (8%)	2 (1%)	25 62
2	C	350/472 (74%)	327 (93%)	18 (5%)	5 (1%)	11 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1674/2166 (77%)	1499 (90%)	151 (9%)	24 (1%)	11 44

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	319	VAL
2	C	391	PRO
1	A	755	LYS
2	C	316	PRO
2	B	451	GLY
1	A	1141	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	830/1029 (81%)	737 (89%)	93 (11%)	6 26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	325/415 (78%)	308 (95%)	17 (5%)	23 55
2	C	318/415 (77%)	295 (93%)	23 (7%)	14 46
All	All	1473/1859 (79%)	1340 (91%)	133 (9%)	9 36

All (133) 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	130	LEU
1	A	177	ARG
1	A	195	LEU
1	A	197	PHE
1	A	227	ARG
1	A	236	THR
1	A	245	ILE
1	A	247	LEU
1	A	264	GLN
1	A	277	HIS
1	A	292	LEU
1	A	304	LEU
1	A	311	LEU
1	A	316	LYS
1	A	346	ASP
1	A	424	LEU
1	A	488	LEU
1	A	499	LYS
1	A	542	ASP
1	A	548	CYS
1	A	558	LEU
1	A	565	HIS
1	A	566	LEU
1	A	595	GLN
1	A	612	LEU
1	A	613	HIS
1	A	617	ARG
1	A	631	LEU
1	A	633	LYS
1	A	634	LEU

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Mol	Chain	Res	Type
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	748	TRP
1	A	750	PHE
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
1	A	816	LEU
1	A	818	ARG
1	A	821	LEU
1	A	841	LEU
1	A	851	THR
1	A	914	THR
1	A	927	ARG
1	A	941	ILE
1	A	964	ARG
1	A	970	ASN
1	A	973	LEU
1	A	977	GLU
1	A	986	TYR
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	1069	ILE
1	A	1071	ARG

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Mol	Chain	Res	Type
1	A	1074	VAL
1	A	1081	ARG
1	A	1090	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	1190	ARG
1	A	1191	LYS
1	A	1197	CYS
1	A	1198	LYS
1	A	1210	TYR
1	A	1218	LEU
2	B	69	LEU
2	B	186	LEU
2	B	231	ILE
2	B	263	TRP
2	B	329	LYS
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	428	LEU
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

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Mol	Chain	Res	Type
2	C	204	LEU
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	284	ARG
2	C	293	PHE
2	C	295	TRP
2	C	300	ILE
2	C	386	ASP
2	C	402	LEU
2	C	453	ILE
2	C	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	354	ASN
1	A	497	GLN
1	A	1134	HIS
2	C	427	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	0.43	0	20,26,29	0.44	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 monosaccharides 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	DCP	A	4003	5	25,29,29	1.67	6 (24%)	37,45,45	1.32	5 (13%)

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	DCP	A	4003	5	-	0/22/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	4003	DCP	C4-N4	3.69	1.42	1.33
6	A	4003	DCP	C2-N1	-3.51	1.32	1.40
6	A	4003	DCP	C1'-N1	-3.02	1.40	1.48
6	A	4003	DCP	C6-C5	2.57	1.41	1.35
6	A	4003	DCP	PB-O1B	2.23	1.58	1.50
6	A	4003	DCP	C2-N3	-2.13	1.32	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4003	DCP	PB-O3A-PA	-2.94	122.72	132.83
6	A	4003	DCP	PB-O3B-PG	-2.80	123.20	132.83
6	A	4003	DCP	O3'-C3'-C4'	2.68	120.36	110.10
6	A	4003	DCP	O3'-C3'-C2'	2.68	120.47	110.90
6	A	4003	DCP	O2-C2-N3	-2.27	118.64	122.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

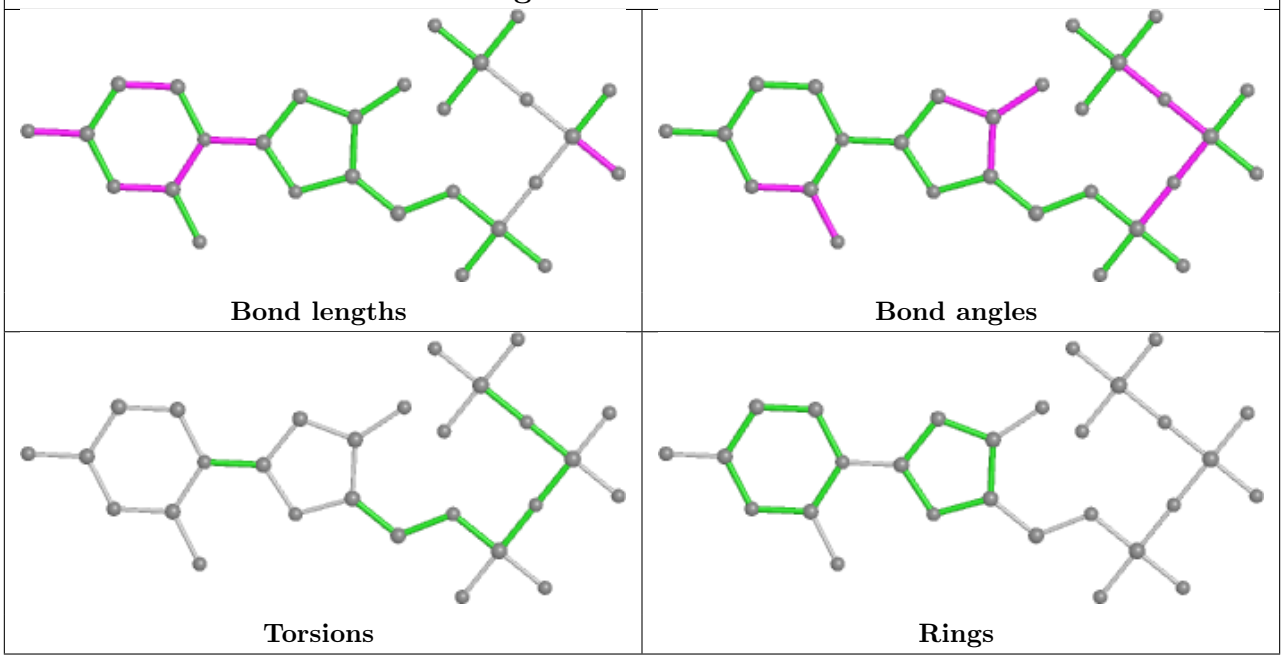
1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	4003	DCP	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand DCP A 4003



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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

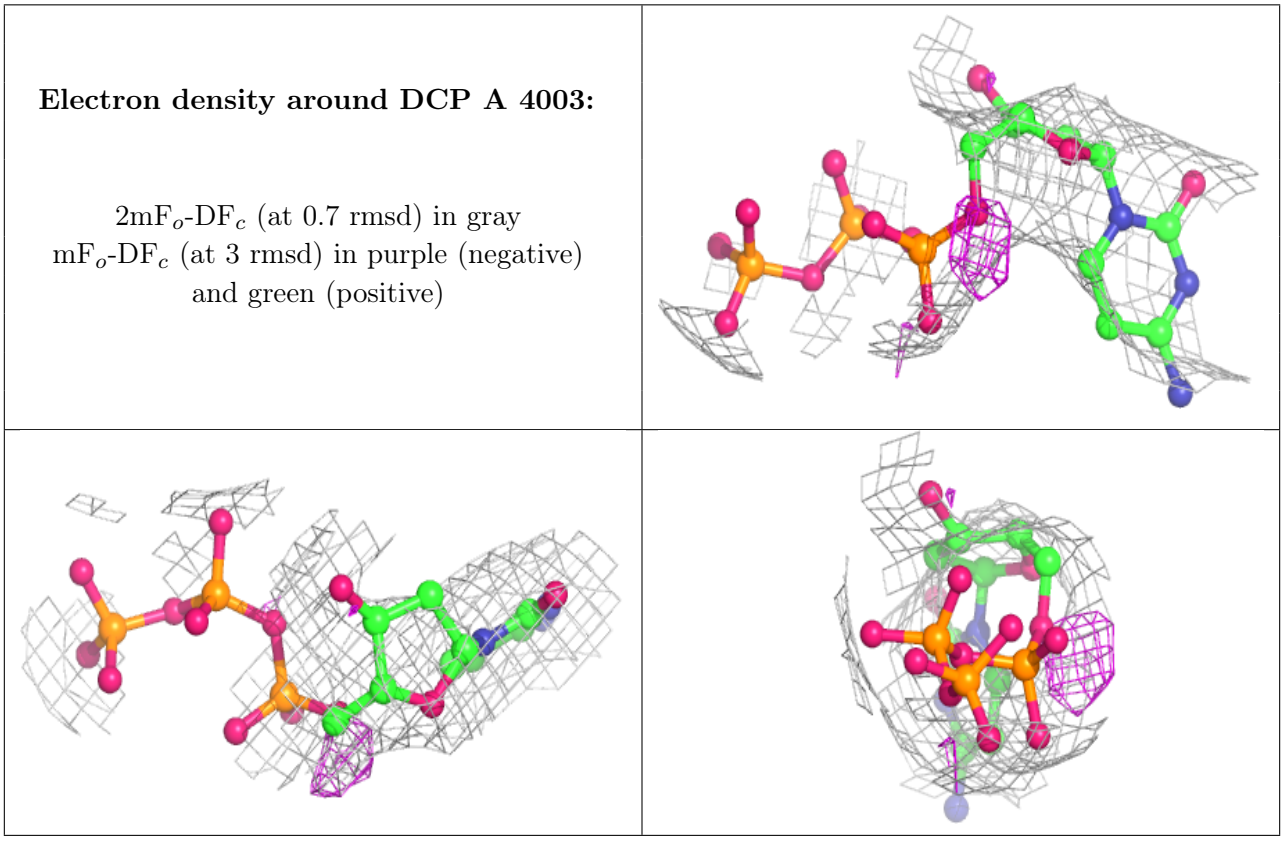
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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 DCP A 4003:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.