



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 08:56 PM EDT

PDB ID : 6AS7  
Title : CRYSTAL STRUCTURE OF THE CATALYTIC CORE OF HUMAN DNA POLYMERASE ALPHA IN TERNARY COMPLEX WITH AN DNA-PRIMED DNA TEMPLATE AND DCTP  
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Deposited on : 2017-08-23  
Resolution : 2.95 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](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

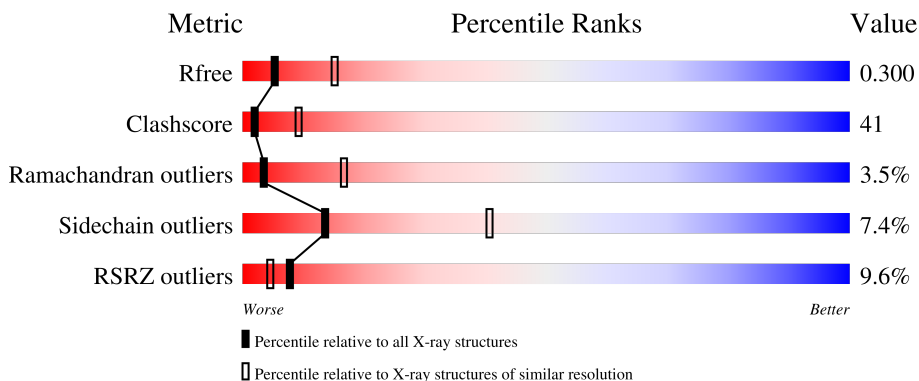
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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  $\geq 3$ , 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	922	 9% 39% 48% 6% 6%
2	B	11	 18% 73% 9%
3	C	13	 15% 77% 8%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 7516 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 alpha catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	870	6996	4504	1171	1280	41	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ALA	VAL	engineered mutation	UNP P09884

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	11	223	106	44	63	10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	13	264	125	52	75	12	0	0	0

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (three-letter code: DCP) (formula: C<sub>9</sub>H<sub>16</sub>N<sub>3</sub>O<sub>13</sub>P<sub>3</sub>).



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

- 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 COBALT (II) ION (three-letter code: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Co	0	0
			1	1		
6	C	1	Total	Co	0	0
			1	1		

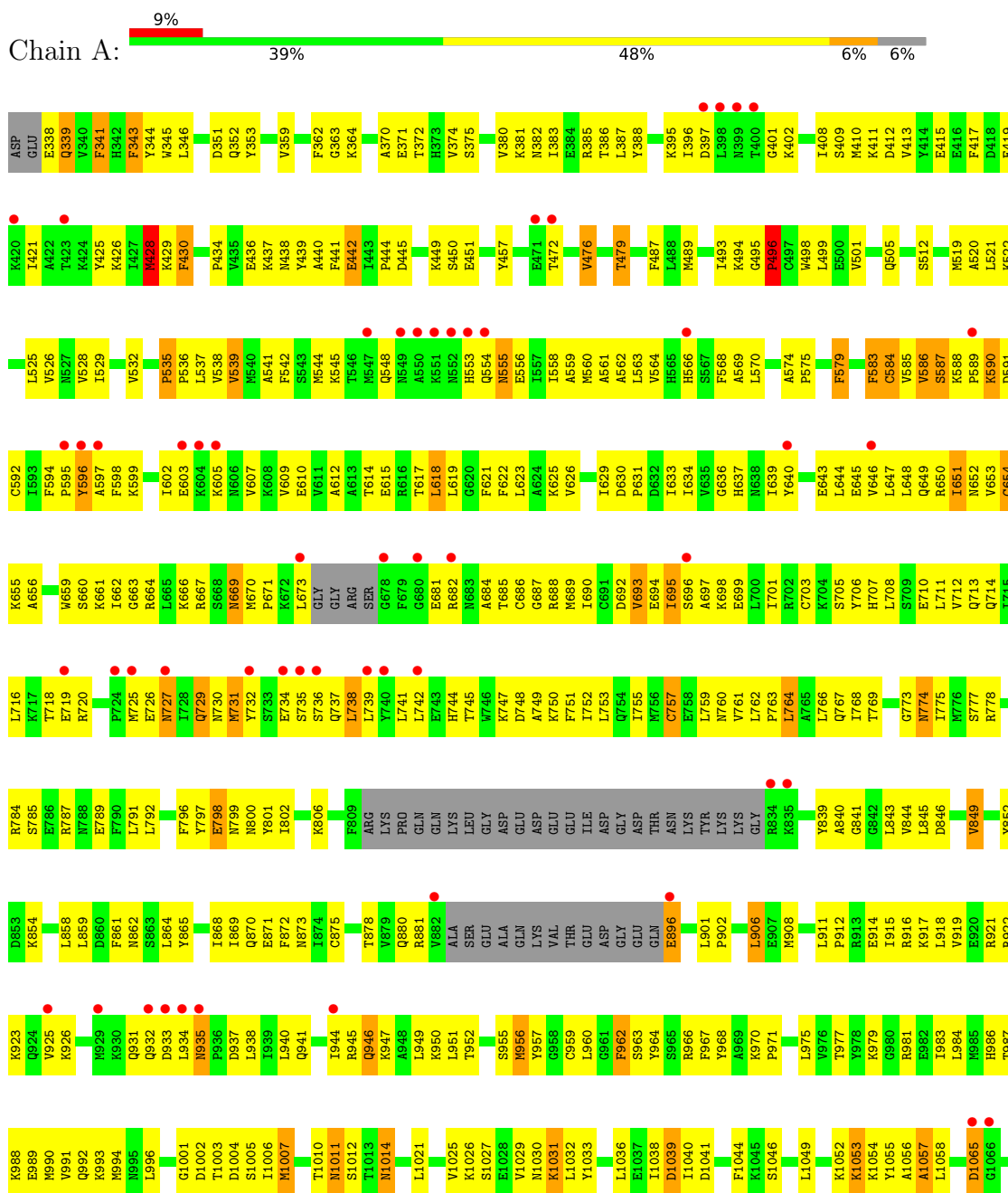
- Molecule 7 is water.

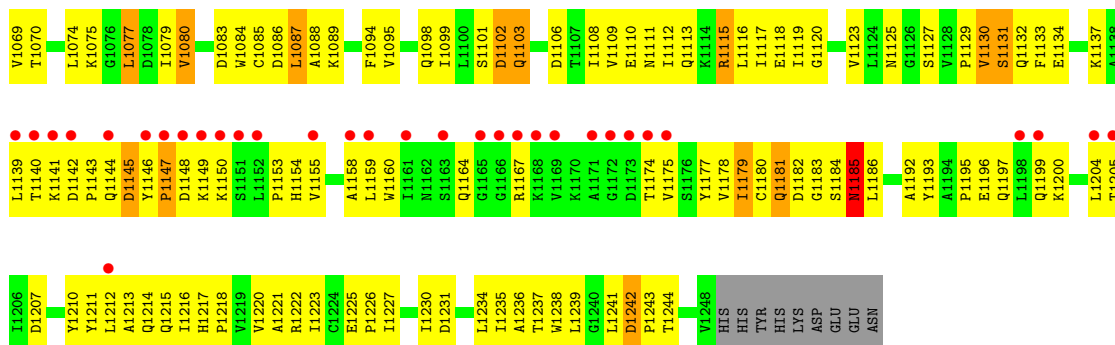
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O	0	0
			1	1		

### 3 Residue-property plots [i](#)

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

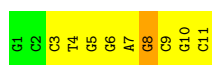
- Molecule 1: DNA polymerase alpha catalytic subunit





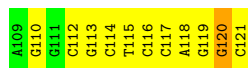
- Molecule 2: DNA (5'-D(\*GP\*CP\*CP\*TP\*GP\*GP\*AP\*GP\*CP\*GP\*C)-3')

Chain B: 18% 73% 9%



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

Chain C: 15% 77% 8%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	151.81Å 151.81Å 113.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.95 46.20 – 2.94	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.20-2.95) 99.5 (46.20-2.94)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.96Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.301 0.263 , 0.300	Depositor DCC
$R_{free}$ test set	1387 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtrriage
Anisotropy	0.070	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	7516	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.50	0/7140	0.74	1/9650 (0.0%)
2	B	0.70	0/250	1.01	1/384 (0.3%)
3	C	0.83	0/296	0.95	0/455
All	All	0.53	0/7686	0.76	2/10489 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	GLY	N-CA-C	-6.00	98.10	113.10
2	B	8	DG	N9-C1'-C2'	5.68	123.39	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	120	DG	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	6996	0	7140	576	0
2	B	223	0	122	24	0
3	C	264	0	146	21	0
4	A	28	0	12	2	0
5	A	2	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	B	1	0	0	0	0
All	All	7516	0	7420	613	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 41.

All (613) 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)
3:C:115:DT:H2''	3:C:116:DC:H5''	1.20	1.19
3:C:118:DA:H2''	3:C:119:DG:H5'	1.22	1.12
2:B:10:DG:C2'	2:B:11:DC:H5'	1.81	1.11
1:A:564:VAL:HG21	1:A:629:ILE:HD13	1.32	1.08
2:B:4:DT:H2''	2:B:5:DG:H5''	1.33	1.08
2:B:7:DA:H2''	2:B:8:DG:H5'	1.37	1.06
2:B:10:DG:H2''	2:B:11:DC:H5'	1.04	1.03
2:B:4:DT:C2'	2:B:5:DG:H5''	1.90	1.01
1:A:574:ALA:HB1	1:A:757:CYS:SG	2.02	1.00
2:B:10:DG:H2''	2:B:11:DC:C5'	1.94	0.98
3:C:115:DT:C2'	3:C:116:DC:H5''	1.93	0.97
1:A:548:GLN:H	1:A:725:MET:HE1	1.24	0.97
1:A:1181:GLN:HE21	1:A:1181:GLN:HA	1.29	0.97
1:A:664:ARG:HD2	1:A:687:GLY:O	1.65	0.97
1:A:1150:LYS:HD2	1:A:1150:LYS:H	1.30	0.95
1:A:859:LEU:HB3	1:A:1038:ILE:HD11	1.45	0.95
1:A:589:PRO:O	1:A:590:LYS:HG3	1.69	0.93
1:A:705:SER:OG	1:A:710:GLU:HG2	1.69	0.92
3:C:115:DT:H2''	3:C:116:DC:C5'	2.01	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1074:LEU:O	1:A:1075:LYS:HD3	1.71	0.91
3:C:118:DA:H2''	3:C:119:DG:C5'	2.02	0.89
1:A:588:LYS:HD2	1:A:592:CYS:O	1.72	0.88
1:A:996:LEU:HD21	1:A:1021:LEU:HD21	1.56	0.88
1:A:915:ILE:HA	1:A:918:LEU:HD12	1.55	0.88
1:A:862:ASN:HA	4:A:1301:DCP:O2G	1.74	0.87
1:A:505:GLN:HG2	1:A:521:LEU:HD21	1.55	0.87
1:A:845:LEU:HD12	1:A:1001:GLY:HA3	1.55	0.86
1:A:652:ASN:HB2	1:A:670:MET:HE3	1.55	0.86
1:A:707:HIS:HB2	1:A:710:GLU:OE1	1.74	0.86
1:A:769:THR:HG23	1:A:774:ASN:OD1	1.74	0.86
1:A:1085:CYS:H	1:A:1215:GLN:NE2	1.73	0.86
1:A:505:GLN:CG	1:A:521:LEU:HD21	2.05	0.86
1:A:388:TYR:CE2	1:A:437:LYS:HE3	2.10	0.85
2:B:7:DA:C2'	2:B:8:DG:H5'	2.05	0.85
1:A:843:LEU:HD12	1:A:844:VAL:N	1.92	0.85
1:A:859:LEU:HD21	1:A:1040:ILE:HD13	1.57	0.84
1:A:541:ALA:O	1:A:562:ALA:HA	1.78	0.84
1:A:636:GLY:C	1:A:639:ILE:HD11	1.97	0.84
1:A:727:ASN:HD22	1:A:727:ASN:N	1.77	0.83
1:A:922:ARG:HH12	1:A:950:LYS:HD2	1.42	0.83
1:A:669:ASN:N	1:A:669:ASN:HD22	1.75	0.81
1:A:1002:ASP:OD2	2:B:11:DC:H5''	1.81	0.81
1:A:370:ALA:O	1:A:372:THR:HG22	1.80	0.80
1:A:762:LEU:HB2	1:A:763:PRO:HD3	1.63	0.79
1:A:1053:LYS:HD3	2:B:10:DG:H1'	1.63	0.79
2:B:5:DG:H2''	2:B:6:DG:O5'	1.82	0.79
1:A:911:LEU:HB3	1:A:912:PRO:HD3	1.63	0.79
1:A:693:VAL:HG21	1:A:752:ILE:HG23	1.62	0.79
2:B:4:DT:C3'	2:B:5:DG:H5''	2.09	0.79
1:A:505:GLN:HE21	1:A:521:LEU:HD11	1.47	0.79
1:A:545:LYS:HZ3	1:A:745:THR:HG23	1.48	0.78
1:A:692:ASP:HB3	1:A:695:ILE:HD12	1.65	0.78
1:A:731:MET:SD	1:A:741:LEU:HB2	2.23	0.78
1:A:1119:ILE:O	1:A:1123:VAL:HG23	1.84	0.77
1:A:1143:PRO:HG2	1:A:1144:GLN:NE2	2.00	0.77
1:A:505:GLN:HB2	1:A:519:MET:HE3	1.67	0.76
1:A:1095:VAL:HG13	1:A:1112:ILE:HD13	1.66	0.75
1:A:415:GLU:HB3	1:A:419:GLU:OE2	1.85	0.75
1:A:548:GLN:N	1:A:725:MET:HE1	2.01	0.75
1:A:662:ILE:HG23	1:A:663:GLY:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:TYR:CD2	1:A:535:PRO:HD3	2.22	0.74
1:A:748:ASP:O	1:A:752:ILE:HG13	1.87	0.74
1:A:1098:GLN:O	1:A:1101:SER:HB3	1.88	0.73
1:A:585:VAL:HG13	1:A:618:LEU:HD11	1.70	0.73
1:A:574:ALA:CB	1:A:757:CYS:SG	2.77	0.72
1:A:859:LEU:HB3	1:A:1038:ILE:CD1	2.20	0.72
1:A:623:LEU:HD11	1:A:651:ILE:HD11	1.69	0.72
1:A:444:PRO:O	1:A:445:ASP:HB2	1.90	0.72
1:A:908:MET:HE1	1:A:916:ARG:HD2	1.72	0.72
1:A:962:PHE:CZ	1:A:964:TYR:HB2	2.25	0.72
1:A:1125:ASN:OD1	1:A:1127:SER:HB2	1.91	0.71
1:A:753:LEU:O	1:A:757:CYS:HB2	1.90	0.71
1:A:919:VAL:O	1:A:923:LYS:HG3	1.91	0.71
1:A:1237:THR:HG23	1:A:1243:PRO:HB3	1.72	0.71
1:A:996:LEU:CD2	1:A:1021:LEU:HD21	2.20	0.71
1:A:1079:ILE:HD11	1:A:1223:ILE:HD11	1.72	0.70
1:A:536:PRO:O	1:A:537:LEU:HD23	1.91	0.70
1:A:922:ARG:NH1	1:A:950:LYS:HB2	2.06	0.70
1:A:417:PHE:HA	1:A:421:ILE:HB	1.73	0.70
1:A:1133:PHE:HB3	1:A:1211:TYR:CZ	2.27	0.70
1:A:1077:LEU:O	1:A:1080:VAL:HG13	1.91	0.70
1:A:1110:GLU:HA	1:A:1110:GLU:OE2	1.93	0.69
1:A:622:PHE:HE2	1:A:647:LEU:HD21	1.57	0.69
1:A:932:GLN:HE21	1:A:932:GLN:HA	1.56	0.69
1:A:1085:CYS:H	1:A:1215:GLN:HE22	1.39	0.69
1:A:1193:TYR:CE1	1:A:1204:LEU:HD21	2.28	0.69
1:A:841:GLY:O	1:A:981:ARG:NH1	2.26	0.69
1:A:1025:VAL:O	1:A:1029:VAL:HG23	1.93	0.69
1:A:694:GLU:O	1:A:698:LYS:HG3	1.92	0.68
1:A:789:GLU:OE2	1:A:966:ARG:HD2	1.93	0.68
2:B:4:DT:H2''	2:B:5:DG:C5'	2.18	0.68
3:C:112:DC:H2''	3:C:113:DG:OP2	1.93	0.68
1:A:932:GLN:HA	1:A:932:GLN:NE2	2.08	0.68
1:A:545:LYS:HE3	1:A:744:HIS:CE1	2.29	0.68
1:A:843:LEU:HD12	1:A:844:VAL:H	1.57	0.68
1:A:1179:ILE:HG22	1:A:1207:ASP:CB	2.25	0.67
1:A:1131:SER:O	1:A:1134:GLU:HG3	1.95	0.67
1:A:388:TYR:HE2	1:A:437:LYS:HE3	1.57	0.67
1:A:595:PRO:HG3	1:A:732:TYR:O	1.95	0.67
1:A:599:LYS:O	1:A:603:GLU:HG2	1.95	0.67
1:A:1038:ILE:CG1	1:A:1039:ASP:N	2.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1143:PRO:HB2	1:A:1159:LEU:HD23	1.76	0.67
1:A:708:LEU:O	1:A:712:VAL:HG23	1.95	0.67
1:A:710:GLU:H	1:A:710:GLU:CD	1.98	0.67
1:A:1130:VAL:O	1:A:1134:GLU:HG2	1.95	0.67
1:A:652:ASN:CB	1:A:670:MET:HE3	2.26	0.66
1:A:438:ASN:OD1	1:A:449:LYS:HG3	1.95	0.66
1:A:621:PHE:O	1:A:625:LYS:HG2	1.94	0.66
1:A:669:ASN:N	1:A:669:ASN:ND2	2.44	0.66
1:A:873:ASN:ND2	1:A:878:THR:HG21	2.10	0.66
1:A:664:ARG:HB2	1:A:687:GLY:HA3	1.75	0.66
1:A:759:LEU:N	1:A:759:LEU:HD23	2.11	0.66
1:A:784:ARG:HH11	1:A:787:ARG:HH12	1.42	0.66
1:A:505:GLN:NE2	1:A:521:LEU:HD11	2.11	0.65
1:A:696:SER:OG	1:A:761:VAL:HG11	1.96	0.65
2:B:6:DG:H2''	2:B:7:DA:O5'	1.96	0.65
1:A:622:PHE:CE2	1:A:647:LEU:HD21	2.31	0.65
1:A:1181:GLN:HB2	1:A:1205:THR:CG2	2.27	0.65
1:A:623:LEU:HD11	1:A:651:ILE:CD1	2.27	0.64
1:A:644:LEU:HD23	1:A:681:GLU:HB3	1.80	0.64
1:A:922:ARG:HH12	1:A:950:LYS:CD	2.11	0.64
1:A:662:ILE:HG23	1:A:663:GLY:H	1.60	0.64
3:C:117:DC:H2''	3:C:118:DA:H5''	1.80	0.64
1:A:505:GLN:HG3	1:A:521:LEU:HD21	1.79	0.64
1:A:873:ASN:O	1:A:902:PRO:HG3	1.96	0.64
3:C:118:DA:C2'	3:C:119:DG:H5'	2.15	0.64
1:A:636:GLY:O	1:A:693:VAL:HG22	1.97	0.64
1:A:859:LEU:CD2	1:A:1040:ILE:HD13	2.27	0.63
1:A:908:MET:CE	1:A:916:ARG:HD2	2.29	0.63
1:A:442:GLU:O	1:A:444:PRO:HD3	1.98	0.63
1:A:1113:GLN:NE2	1:A:1238:TRP:HE1	1.96	0.63
1:A:854:LYS:HG3	1:A:1011:ASN:HD22	1.62	0.63
1:A:568:PHE:HE1	1:A:762:LEU:HD12	1.63	0.63
1:A:1106:ASP:O	1:A:1110:GLU:HG2	1.99	0.63
1:A:1196:GLU:HG3	1:A:1197:GLN:N	2.13	0.63
1:A:410:MET:HG3	1:A:434:PRO:HB3	1.81	0.62
1:A:545:LYS:NZ	1:A:745:THR:HG23	2.15	0.62
1:A:845:LEU:CD1	1:A:1001:GLY:HA3	2.29	0.62
1:A:865:TYR:CD2	4:A:1301:DCP:H2'2	2.35	0.62
1:A:662:ILE:CG2	1:A:663:GLY:H	2.13	0.62
1:A:1227:ILE:HD12	1:A:1227:ILE:N	2.15	0.62
1:A:544:MET:CE	1:A:647:LEU:HD13	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:548:GLN:H	1:A:725:MET:CE	2.05	0.62
1:A:911:LEU:HD11	1:A:956:MET:HG2	1.82	0.62
1:A:951:LEU:O	1:A:955:SER:OG	2.14	0.62
1:A:1116:LEU:HD12	1:A:1238:TRP:CE3	2.35	0.62
1:A:637:HIS:NE2	1:A:708:LEU:N	2.48	0.61
1:A:521:LEU:HB2	1:A:525:LEU:HD11	1.82	0.61
1:A:727:ASN:HD22	1:A:727:ASN:H	1.45	0.61
1:A:1113:GLN:NE2	1:A:1238:TRP:NE1	2.48	0.61
1:A:569:ALA:O	1:A:570:LEU:HD23	1.99	0.61
1:A:1149:LYS:HD3	1:A:1150:LYS:N	2.15	0.61
1:A:344:TYR:O	1:A:363:GLY:HA3	2.01	0.61
1:A:1193:TYR:CD2	1:A:1204:LEU:HD11	2.36	0.61
1:A:662:ILE:CG2	1:A:663:GLY:N	2.64	0.61
1:A:1123:VAL:HG13	1:A:1133:PHE:CZ	2.35	0.61
1:A:585:VAL:HG22	1:A:618:LEU:HD12	1.83	0.61
1:A:727:ASN:N	1:A:727:ASN:ND2	2.47	0.61
1:A:839:TYR:O	3:C:112:DC:H5''	2.01	0.61
1:A:1140:THR:HG23	1:A:1141:LYS:HG3	1.83	0.61
1:A:699:GLU:HG3	1:A:784:ARG:NH2	2.16	0.60
1:A:988:LYS:O	1:A:992:GLN:HG3	2.01	0.60
2:B:6:DG:H2''	2:B:7:DA:C5'	2.31	0.60
1:A:1038:ILE:HG12	1:A:1039:ASP:N	2.17	0.60
1:A:1085:CYS:HB2	1:A:1132:GLN:O	2.02	0.60
1:A:1216:ILE:HG22	1:A:1239:LEU:HD11	1.84	0.60
2:B:7:DA:H2''	2:B:8:DG:C5'	2.25	0.60
1:A:539:VAL:HG21	1:A:568:PHE:CD1	2.37	0.60
1:A:583:PHE:CD1	1:A:583:PHE:C	2.74	0.60
1:A:865:TYR:O	1:A:869:ILE:HG13	2.02	0.60
1:A:645:GLU:HG3	1:A:649:GLN:OE1	2.02	0.60
1:A:564:VAL:HG21	1:A:629:ILE:CD1	2.21	0.60
1:A:1143:PRO:HB2	1:A:1159:LEU:CD2	2.32	0.60
1:A:1196:GLU:HG3	1:A:1197:GLN:H	1.66	0.60
1:A:413:VAL:HA	1:A:472:THR:OG1	2.02	0.59
1:A:382:ASN:ND2	1:A:521:LEU:O	2.28	0.59
1:A:660:SER:C	1:A:662:ILE:H	2.05	0.59
1:A:1116:LEU:HD12	1:A:1238:TRP:HE3	1.66	0.59
1:A:436:GLU:O	1:A:800:ASN:ND2	2.35	0.59
1:A:1038:ILE:CG1	1:A:1039:ASP:H	2.15	0.59
1:A:1237:THR:HG22	1:A:1243:PRO:HG3	1.85	0.59
1:A:409:SER:N	1:A:412:ASP:OD2	2.36	0.59
1:A:875:CYS:HB2	1:A:912:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:117:DC:C2'	3:C:118:DA:H5''	2.32	0.59
1:A:598:PHE:CZ	1:A:602:ILE:HD11	2.37	0.59
1:A:873:ASN:OD1	1:A:908:MET:HA	2.02	0.59
1:A:1095:VAL:HG22	1:A:1112:ILE:HG23	1.85	0.59
1:A:545:LYS:HZ3	1:A:745:THR:CG2	2.16	0.58
1:A:932:GLN:HE21	1:A:932:GLN:CA	2.16	0.58
1:A:963:SER:HA	1:A:968:TYR:CD1	2.37	0.58
1:A:1237:THR:CG2	1:A:1243:PRO:HB3	2.32	0.58
1:A:1180:CYS:HB3	1:A:1205:THR:O	2.03	0.58
1:A:512:SER:HB2	1:A:664:ARG:O	2.04	0.58
1:A:615:GLU:HG2	1:A:654:CYS:SG	2.43	0.58
1:A:636:GLY:CA	1:A:639:ILE:HD11	2.32	0.58
1:A:873:ASN:HD21	1:A:878:THR:HG21	1.67	0.58
1:A:994:MET:HB3	1:A:996:LEU:HD12	1.84	0.58
1:A:934:LEU:HD11	1:A:938:LEU:HD23	1.85	0.58
1:A:1149:LYS:HE3	1:A:1159:LEU:HD12	1.86	0.58
1:A:351:ASP:O	1:A:353:TYR:N	2.37	0.58
1:A:1002:ASP:O	1:A:1003:THR:HB	2.03	0.58
1:A:1038:ILE:HG13	1:A:1039:ASP:H	1.68	0.58
1:A:537:LEU:HD12	1:A:633:ILE:HD12	1.86	0.57
1:A:545:LYS:HE3	1:A:744:HIS:HE1	1.69	0.57
1:A:747:LYS:O	1:A:750:LYS:N	2.34	0.57
1:A:864:LEU:HD22	1:A:1004:ASP:CB	2.35	0.57
2:B:3:DC:H2''	2:B:4:DT:OP2	2.04	0.57
1:A:693:VAL:CG2	1:A:752:ILE:HG23	2.33	0.57
1:A:1098:GLN:O	1:A:1108:ILE:HG12	2.03	0.57
1:A:1120:GLY:HA2	1:A:1212:LEU:HD21	1.87	0.57
1:A:1129:PRO:O	1:A:1131:SER:N	2.38	0.57
1:A:622:PHE:O	1:A:626:VAL:HG23	2.04	0.57
1:A:774:ASN:ND2	1:A:787:ARG:HG2	2.19	0.57
1:A:875:CYS:HB2	1:A:912:PRO:CD	2.34	0.57
3:C:113:DG:H1'	3:C:114:DC:H5''	1.86	0.57
1:A:859:LEU:HD23	1:A:1040:ILE:HA	1.87	0.57
1:A:727:ASN:H	1:A:727:ASN:ND2	2.03	0.57
1:A:731:MET:O	1:A:737:GLN:HB2	2.05	0.57
1:A:806:LYS:HG2	1:A:966:ARG:CZ	2.34	0.57
1:A:990:MET:HE1	1:A:1032:LEU:HD11	1.87	0.57
1:A:1181:GLN:HA	1:A:1181:GLN:NE2	2.09	0.56
1:A:569:ALA:C	1:A:570:LEU:HD23	2.25	0.56
1:A:619:LEU:N	1:A:619:LEU:HD23	2.21	0.56
1:A:644:LEU:CD2	1:A:681:GLU:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:TYR:CD2	1:A:1036:LEU:HB3	2.40	0.56
1:A:1220:VAL:HG12	1:A:1235:ILE:HD13	1.87	0.56
1:A:1210:TYR:CD1	1:A:1214:GLN:HG3	2.40	0.56
1:A:408:ILE:HG22	1:A:409:SER:N	2.19	0.56
1:A:489:MET:HG3	1:A:797:TYR:CE1	2.41	0.56
1:A:623:LEU:HD21	1:A:651:ILE:CD1	2.35	0.56
1:A:1053:LYS:HG2	2:B:10:DG:H4'	1.87	0.56
3:C:118:DA:C2'	3:C:119:DG:C5'	2.81	0.56
1:A:430:PHE:C	1:A:430:PHE:CD1	2.79	0.56
1:A:607:VAL:HB	1:A:609:VAL:HG12	1.87	0.56
1:A:689:MET:HG2	1:A:777:SER:HB3	1.88	0.56
1:A:395:LYS:C	1:A:396:ILE:HD12	2.26	0.56
1:A:1137:LYS:O	1:A:1174:THR:HA	2.05	0.56
1:A:730:ASN:N	1:A:730:ASN:HD22	2.04	0.56
1:A:859:LEU:CB	1:A:1038:ILE:HD11	2.30	0.55
3:C:113:DG:H2''	3:C:114:DC:H5'	1.89	0.55
1:A:476:VAL:HG22	1:A:479:THR:HG23	1.88	0.55
1:A:1087:LEU:H	1:A:1132:GLN:HB3	1.70	0.55
1:A:1115:ARG:O	1:A:1119:ILE:HG12	2.07	0.55
1:A:344:TYR:CE2	1:A:535:PRO:HD3	2.42	0.55
1:A:947:LYS:O	1:A:951:LEU:HG	2.06	0.55
1:A:1142:ASP:HB2	1:A:1145:ASP:OD1	2.06	0.55
1:A:917:LYS:O	1:A:921:ARG:HG3	2.06	0.55
1:A:962:PHE:CD2	3:C:110:DG:H4'	2.42	0.55
1:A:542:PHE:HA	1:A:561:ALA:O	2.07	0.55
1:A:784:ARG:NH1	1:A:787:ARG:HH12	2.03	0.55
1:A:962:PHE:HD1	1:A:963:SER:N	2.05	0.55
1:A:1108:ILE:HG22	1:A:1109:VAL:N	2.21	0.55
1:A:1026:LYS:HG2	1:A:1030:ASN:ND2	2.23	0.54
1:A:732:TYR:CZ	1:A:738:LEU:HD21	2.42	0.54
1:A:747:LYS:NZ	1:A:750:LYS:HD3	2.22	0.54
1:A:864:LEU:HD22	1:A:1004:ASP:HB3	1.89	0.54
1:A:385:ARG:HD2	1:A:457:TYR:CE2	2.43	0.54
1:A:1213:ALA:HB2	1:A:1241:LEU:CD1	2.37	0.54
1:A:921:ARG:O	1:A:925:VAL:HG23	2.06	0.54
1:A:797:TYR:O	1:A:799:ASN:N	2.40	0.54
1:A:505:GLN:CB	1:A:519:MET:HE3	2.35	0.54
1:A:538:VAL:HG22	1:A:566:HIS:HA	1.88	0.54
1:A:1098:GLN:O	1:A:1108:ILE:CG1	2.56	0.54
1:A:386:THR:C	1:A:387:LEU:HD23	2.28	0.54
1:A:990:MET:HG2	1:A:994:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:HIS:O	1:A:554:GLN:HG3	2.08	0.54
2:B:5:DG:H2''	2:B:6:DG:C8	2.42	0.54
2:B:8:DG:H2''	2:B:9:DC:O5'	2.05	0.54
1:A:940:LEU:O	1:A:944:ILE:HG13	2.09	0.53
1:A:637:HIS:N	1:A:639:ILE:HD11	2.23	0.53
1:A:411:LYS:O	1:A:415:GLU:HG3	2.08	0.53
1:A:664:ARG:HD2	1:A:687:GLY:C	2.28	0.53
1:A:983:ILE:HD13	1:A:1036:LEU:CD2	2.39	0.53
1:A:1058:LEU:HB3	1:A:1070:THR:OG1	2.08	0.53
1:A:660:SER:C	1:A:662:ILE:N	2.62	0.53
1:A:872:PHE:HD1	1:A:901:LEU:HD13	1.74	0.53
1:A:1087:LEU:HG	1:A:1216:ILE:HD11	1.90	0.53
1:A:1181:GLN:HB2	1:A:1205:THR:HG23	1.89	0.53
1:A:1231:ASP:OD2	1:A:1234:LEU:HD12	2.09	0.53
1:A:1123:VAL:HG13	1:A:1133:PHE:HZ	1.72	0.53
1:A:957:TYR:O	1:A:960:LEU:HB2	2.08	0.53
3:C:113:DG:H2''	3:C:114:DC:C5'	2.39	0.53
1:A:845:LEU:HD12	1:A:1001:GLY:CA	2.34	0.53
1:A:374:VAL:HG23	1:A:375:SER:O	2.09	0.52
1:A:583:PHE:C	1:A:583:PHE:HD1	2.12	0.52
1:A:731:MET:HA	1:A:737:GLN:CB	2.40	0.52
1:A:731:MET:HA	1:A:737:GLN:HB3	1.92	0.52
1:A:881:ARG:HG2	1:A:881:ARG:HH11	1.75	0.52
1:A:1087:LEU:HB2	1:A:1132:GLN:HE21	1.74	0.52
1:A:568:PHE:CE2	1:A:575:PRO:HD3	2.44	0.52
1:A:583:PHE:CD1	1:A:583:PHE:O	2.62	0.52
1:A:539:VAL:HG13	1:A:633:ILE:HB	1.91	0.52
1:A:962:PHE:CD1	1:A:962:PHE:C	2.82	0.52
1:A:1103:GLN:HB2	1:A:1108:ILE:CD1	2.40	0.52
1:A:659:TRP:CD2	1:A:660:SER:N	2.78	0.52
1:A:727:ASN:O	1:A:731:MET:HG3	2.10	0.52
1:A:1054:LYS:O	1:A:1055:TYR:HB3	2.09	0.52
1:A:559:ALA:O	1:A:560:MET:CG	2.57	0.52
1:A:1053:LYS:HD2	3:C:113:DG:H21	1.74	0.52
1:A:563:LEU:HD23	1:A:579:PHE:CG	2.45	0.52
1:A:970:LYS:HB3	1:A:971:PRO:HD3	1.92	0.52
1:A:596:TYR:O	1:A:597:ALA:HB3	2.09	0.52
1:A:713:GLN:OE1	1:A:713:GLN:HA	2.10	0.52
1:A:806:LYS:HG2	1:A:966:ARG:NH2	2.24	0.52
1:A:1179:ILE:HG22	1:A:1207:ASP:HB3	1.90	0.52
1:A:1231:ASP:O	1:A:1235:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:DG:H2''	2:B:7:DA:H5''	1.91	0.51
1:A:697:ALA:C	1:A:699:GLU:N	2.61	0.51
1:A:1108:ILE:O	1:A:1112:ILE:HG13	2.09	0.51
1:A:396:ILE:CG2	1:A:397:ASP:N	2.73	0.51
1:A:615:GLU:OE1	1:A:654:CYS:SG	2.68	0.51
1:A:1056:ALA:O	1:A:1057:ALA:HB2	2.11	0.51
1:A:1139:LEU:HD11	1:A:1175:VAL:HG23	1.91	0.51
1:A:539:VAL:CG2	1:A:568:PHE:HB3	2.41	0.51
1:A:1182:ASP:OD2	1:A:1193:TYR:OH	2.27	0.51
1:A:558:ILE:C	1:A:558:ILE:HD12	2.31	0.51
1:A:605:LYS:HE2	1:A:739:LEU:HD21	1.93	0.51
1:A:1184:SER:O	1:A:1186:LEU:N	2.43	0.51
1:A:383:ILE:HD13	1:A:487:PHE:HB2	1.93	0.51
1:A:760:ASN:O	1:A:764:LEU:HB2	2.10	0.51
1:A:692:ASP:OD2	1:A:695:ILE:HG13	2.11	0.51
1:A:872:PHE:CE1	1:A:979:LYS:HE2	2.46	0.51
1:A:1184:SER:C	1:A:1185:ASN:HD22	2.13	0.51
1:A:901:LEU:HD23	1:A:975:LEU:HD21	1.93	0.51
1:A:1087:LEU:HA	1:A:1132:GLN:NE2	2.25	0.51
1:A:598:PHE:CE1	1:A:602:ILE:HD11	2.45	0.50
1:A:784:ARG:HH11	1:A:787:ARG:NH1	2.07	0.50
1:A:413:VAL:HG22	1:A:472:THR:HB	1.92	0.50
1:A:660:SER:O	1:A:662:ILE:N	2.45	0.50
1:A:1129:PRO:C	1:A:1131:SER:N	2.64	0.50
1:A:1196:GLU:CG	1:A:1197:GLN:H	2.25	0.50
1:A:395:LYS:HG2	1:A:396:ILE:N	2.26	0.50
1:A:494:LYS:CA	1:A:773:GLY:HA2	2.41	0.50
1:A:619:LEU:HD11	1:A:650:ARG:O	2.11	0.50
1:A:654:CYS:O	1:A:655:LYS:C	2.49	0.50
1:A:558:ILE:HD12	1:A:559:ALA:N	2.27	0.50
1:A:640:TYR:OH	1:A:690:ILE:HB	2.11	0.50
1:A:799:ASN:O	1:A:801:TYR:CD1	2.64	0.50
1:A:859:LEU:HA	1:A:1039:ASP:O	2.12	0.50
1:A:1150:LYS:H	1:A:1150:LYS:CD	2.12	0.50
3:C:114:DC:H2''	3:C:115:DT:O5'	2.11	0.50
3:C:117:DC:H2''	3:C:118:DA:C5'	2.41	0.50
1:A:428:MET:SD	1:A:428:MET:N	2.85	0.50
1:A:539:VAL:HG23	1:A:568:PHE:CB	2.41	0.50
1:A:712:VAL:HG13	1:A:716:LEU:HD12	1.94	0.50
1:A:751:PHE:O	1:A:755:ILE:N	2.43	0.50
1:A:1079:ILE:HD11	1:A:1223:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:TRP:O	1:A:1089:LYS:HE2	2.11	0.50
1:A:1113:GLN:HE21	1:A:1238:TRP:HE1	1.55	0.50
1:A:697:ALA:O	1:A:699:GLU:N	2.45	0.49
1:A:840:ALA:HB1	1:A:981:ARG:NH1	2.27	0.49
1:A:1005:SER:O	1:A:1006:ILE:HD13	2.11	0.49
1:A:1196:GLU:CG	1:A:1197:GLN:N	2.75	0.49
1:A:568:PHE:CE2	1:A:575:PRO:CD	2.96	0.49
1:A:718:THR:HG22	1:A:719:GLU:N	2.26	0.49
1:A:1147:PRO:HG2	1:A:1148:ASP:H	1.77	0.49
1:A:619:LEU:HD13	1:A:651:ILE:HG13	1.93	0.49
1:A:692:ASP:O	1:A:694:GLU:N	2.45	0.49
1:A:589:PRO:O	1:A:590:LYS:CG	2.52	0.49
1:A:1054:LYS:HA	1:A:1075:LYS:O	2.13	0.49
1:A:1227:ILE:N	1:A:1227:ILE:CD1	2.75	0.49
1:A:539:VAL:HG23	1:A:568:PHE:HB3	1.93	0.49
1:A:935:ASN:O	1:A:938:LEU:HB2	2.12	0.49
1:A:388:TYR:O	1:A:476:VAL:HA	2.13	0.49
1:A:559:ALA:O	1:A:560:MET:HG3	2.13	0.49
1:A:963:SER:HA	1:A:968:TYR:CE1	2.48	0.49
1:A:1133:PHE:HB3	1:A:1211:TYR:OH	2.13	0.49
1:A:797:TYR:O	1:A:798:GLU:C	2.51	0.49
1:A:1086:ASP:O	1:A:1088:ALA:N	2.46	0.49
1:A:710:GLU:CD	1:A:710:GLU:N	2.66	0.48
1:A:726:GLU:O	1:A:729:GLN:NE2	2.46	0.48
1:A:1213:ALA:HB2	1:A:1241:LEU:HD13	1.95	0.48
1:A:730:ASN:N	1:A:730:ASN:ND2	2.60	0.48
1:A:1184:SER:O	1:A:1185:ASN:ND2	2.35	0.48
1:A:548:GLN:HA	1:A:554:GLN:O	2.13	0.48
1:A:521:LEU:HD23	1:A:521:LEU:N	2.28	0.48
1:A:623:LEU:HD21	1:A:651:ILE:HD11	1.95	0.48
1:A:962:PHE:CE1	1:A:964:TYR:HB2	2.48	0.48
1:A:1053:LYS:HG2	2:B:10:DG:C4'	2.43	0.48
1:A:660:SER:O	1:A:663:GLY:N	2.47	0.48
1:A:1154:HIS:CE1	1:A:1155:VAL:HG23	2.48	0.48
1:A:705:SER:HG	1:A:710:GLU:HG2	1.74	0.48
1:A:749:ALA:HA	1:A:752:ILE:HD12	1.95	0.48
1:A:769:THR:O	1:A:773:GLY:N	2.44	0.48
1:A:1086:ASP:O	1:A:1087:LEU:C	2.51	0.48
1:A:1131:SER:O	1:A:1134:GLU:CG	2.62	0.48
1:A:630:ASP:HA	1:A:688:ARG:HH12	1.79	0.48
1:A:1149:LYS:HG3	1:A:1159:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1182:ASP:OD2	1:A:1193:TYR:CE1	2.67	0.48
1:A:587:SER:HA	1:A:612:ALA:O	2.13	0.48
1:A:351:ASP:C	1:A:353:TYR:H	2.18	0.47
1:A:568:PHE:CD2	1:A:575:PRO:CD	2.97	0.47
1:A:505:GLN:HB2	1:A:519:MET:CE	2.39	0.47
1:A:498:TRP:CD1	1:A:532:VAL:HB	2.50	0.47
1:A:870:GLN:HE22	1:A:919:VAL:HG21	1.79	0.47
1:A:584:CYS:SG	1:A:742:LEU:HG	2.55	0.47
1:A:646:VAL:O	1:A:650:ARG:HG2	2.15	0.47
1:A:726:GLU:HA	1:A:729:GLN:HE22	1.80	0.47
1:A:986:HIS:HD2	1:A:989:GLU:OE1	1.97	0.47
1:A:1103:GLN:HB2	1:A:1108:ILE:HD12	1.95	0.47
1:A:1143:PRO:HG2	1:A:1144:GLN:HE22	1.74	0.47
1:A:425:TYR:O	1:A:426:LYS:HB2	2.13	0.47
1:A:697:ALA:C	1:A:699:GLU:H	2.18	0.47
1:A:732:TYR:CE2	1:A:738:LEU:HD11	2.50	0.47
1:A:395:LYS:HB2	1:A:408:ILE:HD11	1.97	0.47
1:A:495:GLY:O	1:A:496:PRO:C	2.53	0.47
1:A:797:TYR:O	1:A:800:ASN:N	2.47	0.47
1:A:1150:LYS:HD2	1:A:1150:LYS:N	2.12	0.47
1:A:585:VAL:HG13	1:A:585:VAL:O	2.15	0.47
1:A:615:GLU:CG	1:A:654:CYS:SG	3.02	0.47
1:A:962:PHE:CD1	1:A:963:SER:N	2.83	0.47
1:A:1153:PRO:HB3	1:A:1192:ALA:HB2	1.97	0.47
1:A:555:ASN:O	1:A:650:ARG:HD3	2.15	0.47
1:A:699:GLU:HG3	1:A:784:ARG:HH22	1.80	0.47
1:A:747:LYS:HZ2	1:A:750:LYS:HD3	1.79	0.47
1:A:1149:LYS:HD3	1:A:1150:LYS:HD2	1.97	0.47
1:A:706:TYR:O	1:A:711:LEU:HD11	2.14	0.46
1:A:1112:ILE:HD12	1:A:1230:ILE:CD1	2.45	0.46
1:A:362:PHE:CD1	1:A:687:GLY:HA2	2.50	0.46
1:A:363:GLY:C	1:A:364:LYS:HG2	2.35	0.46
1:A:537:LEU:HD12	1:A:633:ILE:CD1	2.46	0.46
1:A:789:GLU:OE1	1:A:966:ARG:HB2	2.15	0.46
1:A:1087:LEU:CA	1:A:1132:GLN:HE21	2.28	0.46
1:A:1116:LEU:CD1	1:A:1238:TRP:HE3	2.27	0.46
1:A:1158:ALA:HB2	1:A:1175:VAL:HG21	1.96	0.46
1:A:637:HIS:CE1	1:A:708:LEU:H	2.32	0.46
1:A:840:ALA:HB1	1:A:981:ARG:CZ	2.46	0.46
1:A:1014:ASN:C	1:A:1014:ASN:HD22	2.19	0.46
1:A:926:LYS:HD2	1:A:946:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:941:GLN:OE1	1:A:944:ILE:HD12	2.15	0.46
1:A:411:LYS:HE2	1:A:415:GLU:OE2	2.15	0.46
1:A:769:THR:CG2	1:A:774:ASN:OD1	2.58	0.46
1:A:799:ASN:O	1:A:801:TYR:HD1	1.97	0.46
1:A:931:GLN:HB3	1:A:934:LEU:HD22	1.98	0.46
1:A:1102:ASP:O	1:A:1103:GLN:O	2.33	0.46
1:A:617:THR:O	1:A:617:THR:HG22	2.14	0.46
1:A:634:ILE:HD12	1:A:688:ARG:HD2	1.97	0.46
1:A:651:ILE:HG23	1:A:656:ALA:HB3	1.97	0.46
1:A:395:LYS:CA	1:A:408:ILE:HD11	2.46	0.46
1:A:1079:ILE:HA	1:A:1089:LYS:HG2	1.98	0.46
1:A:1083:ASP:OD2	1:A:1083:ASP:N	2.48	0.46
1:A:476:VAL:HG22	1:A:479:THR:CG2	2.46	0.46
1:A:1129:PRO:C	1:A:1131:SER:H	2.18	0.46
1:A:341:PHE:CD1	1:A:501:VAL:HB	2.51	0.45
1:A:563:LEU:HD23	1:A:579:PHE:CD1	2.51	0.45
1:A:1193:TYR:CG	1:A:1204:LEU:HD11	2.50	0.45
1:A:1225:GLU:HB2	1:A:1226:PRO:HD3	1.98	0.45
1:A:343:PHE:CE2	1:A:499:LEU:HD12	2.51	0.45
1:A:450:SER:OG	1:A:451:GLU:N	2.49	0.45
1:A:919:VAL:HG12	1:A:923:LYS:HE3	1.96	0.45
1:A:437:LYS:HB3	1:A:802:ILE:HG12	1.98	0.45
1:A:568:PHE:CE1	1:A:762:LEU:HD12	2.48	0.45
1:A:594:PHE:O	1:A:595:PRO:C	2.55	0.45
1:A:849:VAL:HA	1:A:1049:LEU:O	2.15	0.45
1:A:1242:ASP:OD1	1:A:1244:THR:OG1	2.26	0.45
1:A:345:TRP:HA	1:A:363:GLY:HA3	1.97	0.45
1:A:692:ASP:OD2	1:A:695:ILE:CD1	2.64	0.45
1:A:718:THR:CG2	1:A:719:GLU:N	2.80	0.45
1:A:989:GLU:O	1:A:993:LYS:HG3	2.17	0.45
1:A:1237:THR:HG22	1:A:1243:PRO:CG	2.47	0.45
1:A:631:PRO:HD2	1:A:688:ARG:NH1	2.31	0.45
1:A:922:ARG:HH12	1:A:950:LYS:CG	2.29	0.45
1:A:1069:VAL:HG12	1:A:1070:THR:N	2.31	0.45
1:A:1160:TRP:CZ2	1:A:1164:GLN:NE2	2.82	0.45
2:B:6:DG:C2'	2:B:7:DA:O5'	2.63	0.45
1:A:631:PRO:HG2	1:A:688:ARG:HD3	1.99	0.45
1:A:648:LEU:HD21	1:A:662:ILE:CD1	2.47	0.45
1:A:666:LYS:C	1:A:667:ARG:HG3	2.36	0.45
1:A:738:LEU:HA	1:A:738:LEU:HD23	1.77	0.45
1:A:840:ALA:HB3	1:A:981:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:ARG:HA	1:A:1225:GLU:HG3	1.97	0.45
3:C:117:DC:H1'	3:C:118:DA:H5''	1.98	0.45
1:A:359:VAL:HG23	1:A:383:ILE:HD12	1.99	0.45
1:A:792:LEU:HD12	1:A:967:PHE:CD1	2.51	0.45
1:A:556:GLU:HA	1:A:615:GLU:OE2	2.17	0.45
1:A:1179:ILE:HG22	1:A:1207:ASP:HB2	1.99	0.45
1:A:911:LEU:O	1:A:914:GLU:HB2	2.17	0.44
1:A:1134:GLU:OE2	1:A:1195:PRO:HB3	2.17	0.44
1:A:673:LEU:HB2	1:A:681:GLU:OE2	2.18	0.44
1:A:796:PHE:O	1:A:801:TYR:HB2	2.16	0.44
1:A:1236:ALA:O	1:A:1237:THR:C	2.55	0.44
1:A:662:ILE:HG23	1:A:684:ALA:O	2.16	0.44
1:A:748:ASP:O	1:A:752:ILE:CG1	2.64	0.44
1:A:947:LYS:HG2	1:A:951:LEU:HD11	1.98	0.44
1:A:1027:SER:O	1:A:1031:LYS:HB2	2.17	0.44
1:A:545:LYS:HZ3	1:A:745:THR:CB	2.31	0.44
1:A:791:LEU:HD23	1:A:956:MET:HE1	1.99	0.44
1:A:896:GLU:C	1:A:896:GLU:CD	2.76	0.44
1:A:544:MET:HE3	1:A:647:LEU:HD13	1.98	0.44
1:A:843:LEU:HB2	1:A:981:ARG:HG2	1.99	0.44
1:A:385:ARG:HD2	1:A:457:TYR:CZ	2.53	0.44
1:A:545:LYS:CE	1:A:744:HIS:CE1	3.00	0.44
1:A:844:VAL:HG11	1:A:1052:LYS:HD3	1.98	0.44
1:A:410:MET:HA	1:A:410:MET:CE	2.47	0.44
1:A:861:PHE:HA	1:A:1038:ILE:HA	2.00	0.44
1:A:935:ASN:C	1:A:935:ASN:HD22	2.20	0.44
1:A:1137:LYS:HE3	1:A:1177:TYR:OH	2.17	0.44
1:A:703:CYS:SG	1:A:714:GLN:NE2	2.91	0.44
1:A:1113:GLN:HB2	1:A:1238:TRP:CZ2	2.53	0.44
1:A:568:PHE:CD2	1:A:575:PRO:HD3	2.53	0.43
1:A:586:VAL:O	1:A:612:ALA:HB3	2.18	0.43
1:A:791:LEU:HD23	1:A:956:MET:CE	2.48	0.43
1:A:1094:PHE:CD1	1:A:1094:PHE:C	2.91	0.43
1:A:522:LYS:H	1:A:525:LEU:HD12	1.82	0.43
1:A:1117:ILE:HG22	1:A:1118:GLU:N	2.32	0.43
1:A:1146:TYR:CD1	1:A:1155:VAL:HG11	2.53	0.43
1:A:579:PHE:CD1	1:A:579:PHE:N	2.86	0.43
1:A:594:PHE:C	1:A:595:PRO:O	2.56	0.43
1:A:699:GLU:CG	1:A:784:ARG:HH22	2.31	0.43
1:A:870:GLN:O	1:A:871:GLU:C	2.57	0.43
1:A:946:GLN:HE21	1:A:946:GLN:HB3	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1200:LYS:HB3	1:A:1200:LYS:HE2	1.72	0.43
1:A:487:PHE:HZ	1:A:526:VAL:HG11	1.83	0.43
1:A:945:ARG:HG2	1:A:949:LEU:CD1	2.47	0.43
1:A:563:LEU:HD12	1:A:563:LEU:N	2.34	0.43
1:A:1053:LYS:CD	2:B:10:DG:H1'	2.42	0.43
1:A:692:ASP:CB	1:A:695:ILE:HD12	2.44	0.43
1:A:732:TYR:CE1	1:A:738:LEU:HD21	2.54	0.43
1:A:911:LEU:CB	1:A:912:PRO:HD3	2.44	0.43
1:A:1086:ASP:HB2	1:A:1132:GLN:HA	1.99	0.43
1:A:1213:ALA:HB2	1:A:1241:LEU:HD11	2.00	0.43
1:A:682:ARG:HG2	1:A:682:ARG:HH11	1.84	0.43
1:A:906:LEU:HD12	1:A:906:LEU:H	1.82	0.43
1:A:987:THR:O	1:A:991:VAL:HG23	2.18	0.43
1:A:449:LYS:O	1:A:450:SER:HB2	2.18	0.43
1:A:585:VAL:HG13	1:A:618:LEU:CD1	2.43	0.43
1:A:806:LYS:HB3	1:A:806:LYS:HE2	1.64	0.43
1:A:1010:THR:C	1:A:1012:SER:H	2.22	0.43
1:A:1243:PRO:O	1:A:1244:THR:C	2.57	0.43
1:A:545:LYS:HE2	1:A:744:HIS:ND1	2.33	0.43
3:C:115:DT:OP1	3:C:115:DT:C4'	2.66	0.43
1:A:659:TRP:CE3	1:A:660:SER:HA	2.54	0.43
1:A:695:ILE:HG13	1:A:695:ILE:H	1.55	0.43
1:A:845:LEU:HB2	1:A:1001:GLY:N	2.33	0.42
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.79	0.42
1:A:653:VAL:C	1:A:655:LYS:H	2.22	0.42
1:A:767:GLN:O	1:A:768:ILE:C	2.57	0.42
1:A:858:LEU:HD23	1:A:1041:ASP:HB3	2.01	0.42
1:A:1084:TRP:HZ3	1:A:1215:GLN:HA	1.84	0.42
1:A:1241:LEU:O	1:A:1243:PRO:HD3	2.19	0.42
1:A:602:ILE:CG2	1:A:609:VAL:HG13	2.50	0.42
1:A:695:ILE:HA	1:A:698:LYS:HD2	2.01	0.42
1:A:494:LYS:HA	1:A:773:GLY:CA	2.50	0.42
1:A:1215:GLN:C	1:A:1218:PRO:HD2	2.40	0.42
3:C:120:DG:H2''	3:C:121:DC:OP2	2.19	0.42
1:A:380:VAL:HG22	1:A:520:ALA:HB3	2.02	0.42
1:A:1141:LYS:HB3	1:A:1145:ASP:CB	2.49	0.42
1:A:344:TYR:CE1	1:A:346:LEU:HD21	2.54	0.42
1:A:395:LYS:HA	1:A:408:ILE:HD11	2.02	0.42
1:A:396:ILE:HG22	1:A:397:ASP:N	2.34	0.42
1:A:498:TRP:HB3	1:A:529:ILE:HD11	2.01	0.42
1:A:544:MET:HE1	1:A:647:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:563:LEU:HB3	1:A:579:PHE:CB	2.49	0.42
1:A:852:TYR:O	1:A:1046:SER:HA	2.20	0.42
1:A:1087:LEU:CB	1:A:1132:GLN:HE21	2.32	0.42
1:A:1217:HIS:O	1:A:1221:ALA:HB2	2.19	0.42
1:A:494:LYS:HA	1:A:773:GLY:HA2	2.01	0.42
1:A:598:PHE:O	1:A:602:ILE:HG13	2.20	0.42
1:A:1007:MET:CE	1:A:1044:PHE:HE2	2.31	0.42
1:A:769:THR:HA	1:A:774:ASN:OD1	2.20	0.42
1:A:775:ILE:O	1:A:778:ARG:HB2	2.19	0.42
1:A:1085:CYS:O	1:A:1086:ASP:C	2.56	0.42
1:A:1086:ASP:O	1:A:1089:LYS:N	2.53	0.42
1:A:1149:LYS:HE3	1:A:1159:LEU:CD1	2.49	0.42
1:A:401:GLY:O	1:A:402:LYS:HD3	2.19	0.42
1:A:539:VAL:CG2	1:A:568:PHE:CB	2.98	0.42
1:A:553:HIS:O	1:A:553:HIS:CG	2.73	0.42
1:A:1141:LYS:HB3	1:A:1145:ASP:HB2	2.02	0.42
1:A:650:ARG:NH1	1:A:653:VAL:HG21	2.35	0.42
1:A:1095:VAL:O	1:A:1099:ILE:HG13	2.20	0.42
1:A:659:TRP:CG	1:A:660:SER:N	2.88	0.41
1:A:1127:SER:O	1:A:1129:PRO:HD3	2.20	0.41
1:A:338:GLU:O	1:A:339:GLN:HB2	2.19	0.41
1:A:440:ALA:C	1:A:441:PHE:CG	2.94	0.41
1:A:619:LEU:CD1	1:A:650:ARG:O	2.68	0.41
1:A:637:HIS:CD2	1:A:708:LEU:HB2	2.55	0.41
1:A:938:LEU:O	1:A:941:GLN:HB2	2.19	0.41
1:A:945:ARG:HG2	1:A:949:LEU:HD12	2.03	0.41
1:A:992:GLN:C	1:A:994:MET:N	2.74	0.41
1:A:708:LEU:HD23	1:A:720:ARG:NE	2.36	0.41
1:A:871:GLU:HG2	1:A:872:PHE:CE2	2.56	0.41
1:A:1069:VAL:CG1	1:A:1070:THR:N	2.84	0.41
1:A:1181:GLN:HE21	1:A:1181:GLN:CA	2.15	0.41
1:A:381:LYS:HE2	1:A:381:LYS:HB3	1.57	0.41
1:A:387:LEU:HD22	1:A:479:THR:HA	2.02	0.41
1:A:440:ALA:O	1:A:441:PHE:CD1	2.74	0.41
1:A:692:ASP:OD2	1:A:695:ILE:HD11	2.21	0.41
1:A:493:ILE:HG12	1:A:528:VAL:CG2	2.51	0.41
1:A:865:TYR:OH	1:A:977:THR:HG22	2.20	0.41
1:A:548:GLN:NE2	1:A:554:GLN:O	2.54	0.41
1:A:696:SER:CB	1:A:761:VAL:HG11	2.51	0.41
1:A:864:LEU:O	1:A:868:ILE:HG13	2.21	0.41
1:A:984:LEU:O	1:A:984:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:DT:C3'	2:B:5:DG:C5'	2.92	0.41
1:A:871:GLU:OE1	1:A:1033:TYR:HB3	2.20	0.41
1:A:408:ILE:HA	1:A:412:ASP:OD2	2.20	0.40
1:A:639:ILE:HG22	1:A:644:LEU:HB2	2.03	0.40
1:A:922:ARG:NH1	1:A:950:LYS:CB	2.82	0.40
1:A:1148:ASP:OD1	1:A:1148:ASP:O	2.39	0.40
1:A:408:ILE:CG2	1:A:409:SER:N	2.82	0.40
1:A:734:GLU:OE2	1:A:736:SER:HB2	2.21	0.40
1:A:859:LEU:HD11	1:A:1025:VAL:HB	2.02	0.40
1:A:697:ALA:O	1:A:698:LYS:C	2.56	0.40
1:A:992:GLN:C	1:A:994:MET:H	2.24	0.40
1:A:1217:HIS:N	1:A:1218:PRO:CD	2.84	0.40
1:A:555:ASN:HD22	1:A:555:ASN:HA	1.60	0.40
1:A:951:LEU:HG	1:A:951:LEU:H	1.67	0.40
1:A:1077:LEU:HD12	1:A:1079:ILE:HD12	2.02	0.40
1:A:1085:CYS:N	1:A:1215:GLN:HE22	2.11	0.40
1:A:1111:ASN:N	1:A:1111:ASN:HD22	2.19	0.40
1:A:439:TYR:CZ	1:A:441:PHE:HB2	2.56	0.40
1:A:785:SER:HA	1:A:959:CYS:SG	2.62	0.40
1:A:1029:VAL:O	1:A:1030:ASN:C	2.60	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	862/922 (94%)	723 (84%)	109 (13%)	30 (4%)	<b>3</b>   <b>17</b>

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	GLN

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Mol	Chain	Res	Type
1	A	352	GLN
1	A	590	LYS
1	A	1103	GLN
1	A	1185	ASN
1	A	442	GLU
1	A	479	THR
1	A	654	CYS
1	A	693	VAL
1	A	774	ASN
1	A	798	GLU
1	A	1065	ASP
1	A	1130	VAL
1	A	496	PRO
1	A	952	THR
1	A	1087	LEU
1	A	1167	ARG
1	A	371	GLU
1	A	643	GLU
1	A	661	LYS
1	A	731	MET
1	A	1031	LYS
1	A	1057	ALA
1	A	766	LEU
1	A	849	VAL
1	A	906	LEU
1	A	428	MET
1	A	671	PRO
1	A	1147	PRO
1	A	701	ILE

### 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	783/827 (95%)	725 (93%)	58 (7%)	<b>13</b> 41

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	PHE
1	A	343	PHE
1	A	428	MET
1	A	429	LYS
1	A	430	PHE
1	A	476	VAL
1	A	496	PRO
1	A	535	PRO
1	A	539	VAL
1	A	555	ASN
1	A	579	PHE
1	A	583	PHE
1	A	584	CYS
1	A	586	VAL
1	A	587	SER
1	A	591	ASP
1	A	596	TYR
1	A	610	GLU
1	A	614	THR
1	A	618	LEU
1	A	651	ILE
1	A	669	ASN
1	A	685	THR
1	A	686	CYS
1	A	695	ILE
1	A	727	ASN
1	A	729	GLN
1	A	735	SER
1	A	738	LEU
1	A	757	CYS
1	A	764	LEU
1	A	846	ASP
1	A	880	GLN
1	A	896	GLU
1	A	933	ASP
1	A	935	ASN
1	A	937	ASP
1	A	946	GLN
1	A	956	MET
1	A	962	PHE
1	A	1007	MET
1	A	1011	ASN

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Mol	Chain	Res	Type
1	A	1014	ASN
1	A	1039	ASP
1	A	1053	LYS
1	A	1065	ASP
1	A	1077	LEU
1	A	1080	VAL
1	A	1102	ASP
1	A	1115	ARG
1	A	1131	SER
1	A	1145	ASP
1	A	1178	VAL
1	A	1179	ILE
1	A	1181	GLN
1	A	1185	ASN
1	A	1199	GLN
1	A	1242	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	354	ASN
1	A	475	HIS
1	A	505	GLN
1	A	548	GLN
1	A	554	GLN
1	A	555	ASN
1	A	669	ASN
1	A	683	ASN
1	A	714	GLN
1	A	727	ASN
1	A	729	GLN
1	A	730	ASN
1	A	760	ASN
1	A	770	ASN
1	A	807	GLN
1	A	870	GLN
1	A	880	GLN
1	A	897	GLN
1	A	931	GLN
1	A	932	GLN
1	A	935	ASN
1	A	986	HIS

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Mol	Chain	Res	Type
1	A	1011	ASN
1	A	1014	ASN
1	A	1023	ASN
1	A	1098	GLN
1	A	1111	ASN
1	A	1113	GLN
1	A	1132	GLN
1	A	1144	GLN
1	A	1154	HIS
1	A	1181	GLN
1	A	1185	ASN
1	A	1199	GLN
1	A	1215	GLN
1	A	1245	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](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 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
4	DCP	A	1301	5	25,29,29	1.46	3 (12%)	37,45,45	1.34	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
4	DCP	A	1301	5	-	1/22/34/34	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	DCP	PG-O1G	3.14	1.60	1.50
4	A	1301	DCP	PB-O1B	3.00	1.61	1.50
4	A	1301	DCP	C4-N4	2.20	1.39	1.33

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DCP	PB-O3B-PG	-4.69	116.73	132.83
4	A	1301	DCP	PB-O3A-PA	-4.18	118.47	132.83
4	A	1301	DCP	O4'-C1'-N1	2.08	111.58	107.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1301	DCP	PB-O3B-PG-O3G

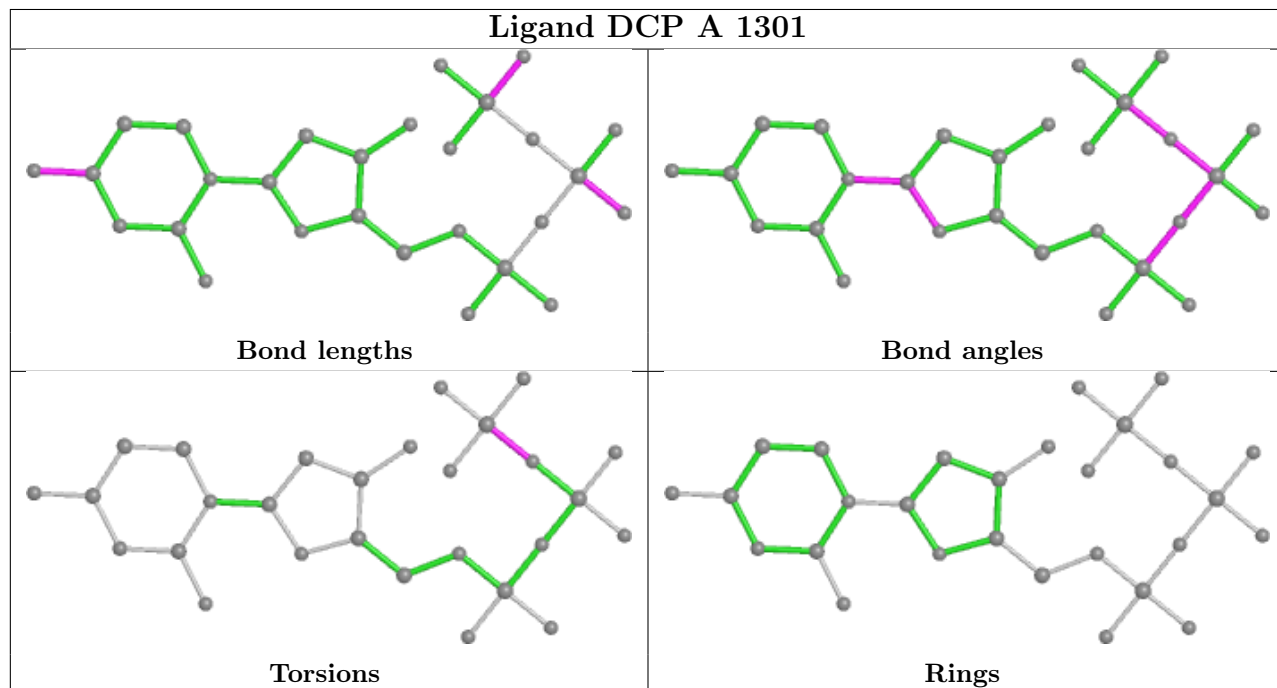
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DCP	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	870/922 (94%)	0.42	86 (9%) <b>7</b> <b>4</b>	7, 52, 113, 138	0
2	B	11/11 (100%)	-0.09	0 <b>100</b> <b>100</b>	26, 43, 66, 68	0
3	C	13/13 (100%)	-0.08	0 <b>100</b> <b>100</b>	22, 41, 72, 86	0
All	All	894/946 (94%)	0.40	86 (9%) <b>8</b> <b>4</b>	7, 52, 112, 138	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	551	LYS	9.6
1	A	1149	LYS	9.1
1	A	399	ASN	7.3
1	A	1172	GLY	5.9
1	A	1146	TYR	5.9
1	A	1165	GLY	5.7
1	A	597	ALA	5.6
1	A	1140	THR	5.3
1	A	1167	ARG	5.0
1	A	1151	SER	4.9
1	A	1173	ASP	4.9
1	A	596	TYR	4.8
1	A	1139	LEU	4.7
1	A	420	LYS	4.7
1	A	1171	ALA	4.5
1	A	678	GLY	4.5
1	A	550	ALA	4.2
1	A	1166	GLY	4.1
1	A	1199	GLN	4.1
1	A	735	SER	4.0
1	A	934	LEU	4.0
1	A	724	PRO	3.9
1	A	725	MET	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	471	GLU	3.8
1	A	397	ASP	3.8
1	A	1152	LEU	3.7
1	A	646	VAL	3.7
1	A	1066	GLY	3.7
1	A	933	ASP	3.6
1	A	1144	GLN	3.6
1	A	1175	VAL	3.6
1	A	472	THR	3.6
1	A	400	THR	3.5
1	A	734	GLU	3.4
1	A	549	ASN	3.4
1	A	1161	ILE	3.3
1	A	554	GLN	3.3
1	A	1148	ASP	3.3
1	A	1147	PRO	3.3
1	A	1158	ALA	3.2
1	A	925	VAL	3.1
1	A	566	HIS	3.1
1	A	603	GLU	3.1
1	A	1142	ASP	3.0
1	A	547	MET	3.0
1	A	732	TYR	2.9
1	A	835	LYS	2.9
1	A	553	HIS	2.8
1	A	1159	LEU	2.8
1	A	1163	SER	2.8
1	A	1141	LYS	2.8
1	A	1169	VAL	2.7
1	A	1168	LYS	2.7
1	A	719	GLU	2.6
1	A	896	GLU	2.6
1	A	882	VAL	2.6
1	A	1150	LYS	2.6
1	A	604	LYS	2.6
1	A	605	LYS	2.6
1	A	1205	THR	2.5
1	A	680	GLY	2.5
1	A	1204	LEU	2.5
1	A	736	SER	2.4
1	A	834	ARG	2.4
1	A	727	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	398	LEU	2.4
1	A	589	PRO	2.4
1	A	552	ASN	2.3
1	A	740	TYR	2.3
1	A	696	SER	2.2
1	A	1174	THR	2.2
1	A	423	THR	2.2
1	A	932	GLN	2.1
1	A	595	PRO	2.1
1	A	1065	ASP	2.1
1	A	935	ASN	2.1
1	A	673	LEU	2.1
1	A	682	ARG	2.1
1	A	929	MET	2.1
1	A	1198	LEU	2.1
1	A	944	ILE	2.1
1	A	640	TYR	2.0
1	A	742	LEU	2.0
1	A	739	LEU	2.0
1	A	1155	VAL	2.0
1	A	1212	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

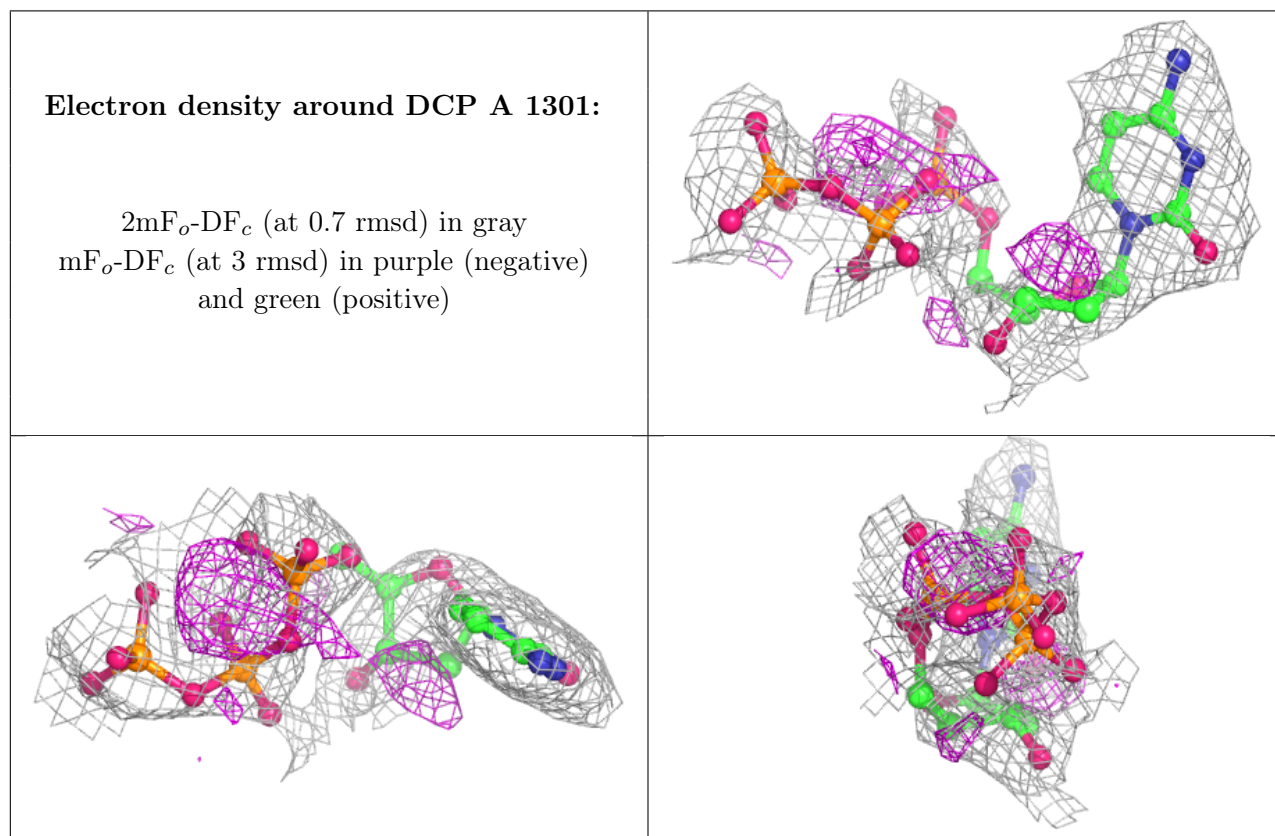
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DCP	A	1301	28/28	0.84	0.30	42,85,136,136	0
5	MG	A	1302	1/1	0.93	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	CO	B	101	1/1	0.94	0.15	62,62,62,62	0
6	CO	C	401	1/1	0.96	0.19	73,73,73,73	0
5	MG	A	1303	1/1	0.97	0.15	51,51,51,51	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.