



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:55 AM UTC

PDB ID : 6AS7 / pdb_00006as7
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

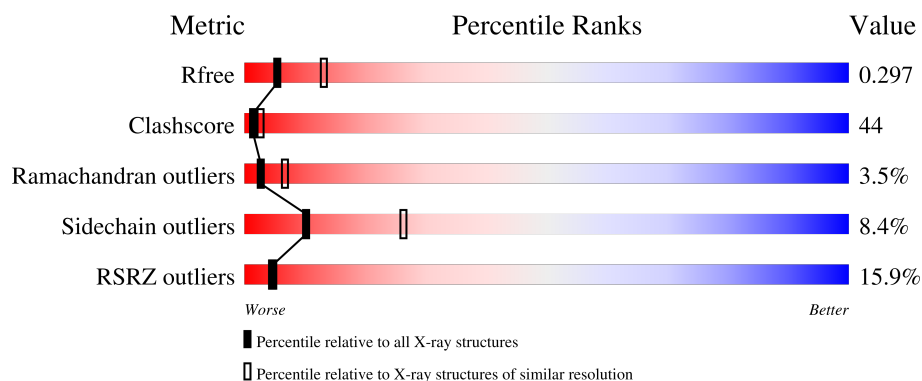
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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

Mol	Chain	Length	Quality of chain
1	A	922	15% 35% 50% 9% 6%
2	B	11	18% 45% 36%
3	C	13	8% 8% 69% 23%

2 Entry composition

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
1	A	870	Total	C	N	O	S	0	0	0
			6996	4504	1171	1280	41			

There is a discrepancy between the modelled and reference sequences:

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

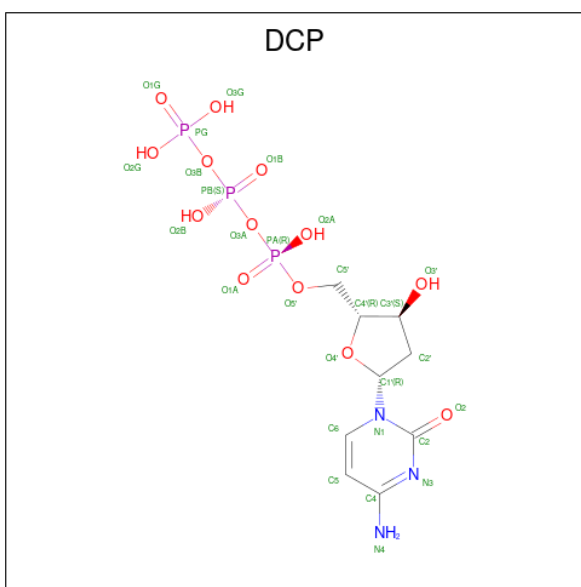
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*CP*CP*TP*GP*GP*AP*GP*CP*GP*C)-3').

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

- 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
3	C	13	Total	C	N	O	P	0	0	0
			264	125	52	75	12			

- Molecule 4 is 2'-DEOXYCYTIDINE-5'-TRIPHOSPHATE (CCD ID: DCP) (formula: C₉H₁₆N₃O₁₃P₃).



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 (CCD ID: MG) (formula: Mg).

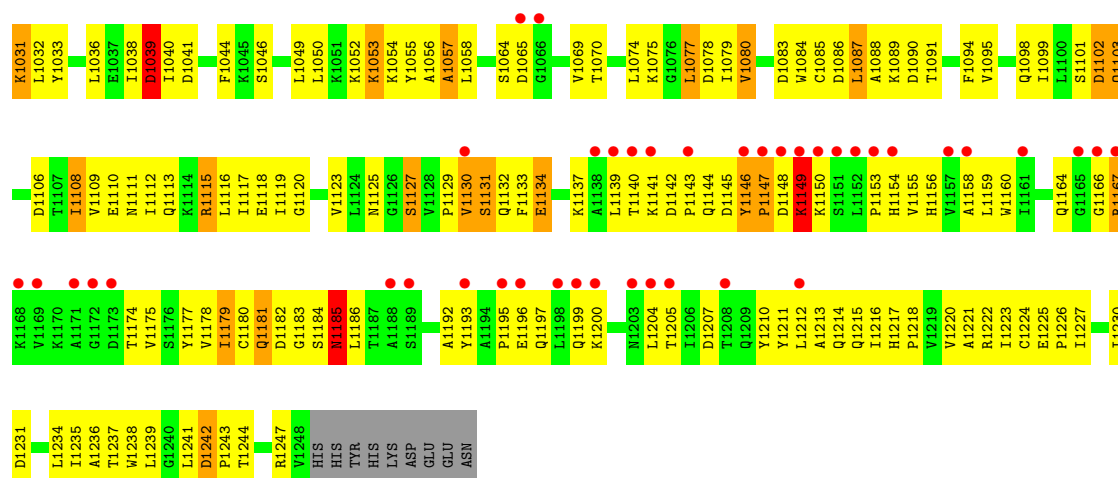
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		

- Molecule 6 is COBALT (II) ION (CCD ID: 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		

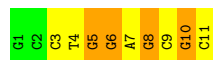
- Molecule 7 is water.

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



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

Chain B: 18% 45% 36%



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

Chain C: 8% 69% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	151.81Å 151.81Å 113.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.20 – 2.95 46.20 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.6 (46.20-2.95) 99.6 (46.20-2.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.96Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.259 , 0.301 0.260 , 0.297	Depositor DCC
R_{free} test set	1387 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7516	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [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	0.61	2/7140 (0.0%)	1.13	49/9650 (0.5%)
2	B	0.46	0/250	1.23	4/384 (1.0%)
3	C	0.51	0/296	1.03	3/455 (0.7%)
All	All	0.60	2/7686 (0.0%)	1.13	56/10489 (0.5%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	ILE	CA-CB	5.29	1.59	1.53
1	A	756	MET	SD-CE	5.10	1.92	1.79

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1183	GLY	N-CA-C	-11.05	98.10	115.67
1	A	662	ILE	N-CA-C	-9.68	101.93	110.74
2	B	6	DG	C2'-C3'-O3'	8.46	124.19	111.50
1	A	525	LEU	N-CA-C	-7.97	103.57	113.38
1	A	1149	LYS	N-CA-C	7.91	119.53	111.07
1	A	398	LEU	N-CA-C	7.90	119.97	111.36
1	A	687	GLY	N-CA-C	-7.33	105.13	114.37
3	C	114	DC	C2'-C3'-O3'	7.22	122.33	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	564	VAL	N-CA-C	7.15	118.61	108.17
2	B	5	DG	C2'-C3'-O3'	7.13	122.20	111.50
1	A	743	GLU	N-CA-C	-7.11	104.08	112.89
1	A	630	ASP	CA-C-N	6.97	127.22	119.90
1	A	630	ASP	C-N-CA	6.97	127.22	119.90
1	A	1021	LEU	N-CA-C	-6.97	103.70	111.71
1	A	533	SER	CA-C-N	-6.84	113.33	120.38
1	A	533	SER	C-N-CA	-6.84	113.33	120.38
1	A	441	PHE	N-CA-C	6.62	119.01	109.14
2	B	8	DG	N9-C1'-C2'	6.60	123.39	113.50
1	A	897	GLN	N-CA-C	-6.56	97.64	108.07
1	A	1078	ASP	N-CA-C	-6.45	103.53	111.33
2	B	10	DG	C2'-C3'-O3'	-6.40	101.91	111.50
1	A	756	MET	N-CA-C	-6.37	103.95	111.03
1	A	421	ILE	N-CA-C	6.29	116.40	110.30
1	A	728	ILE	N-CA-C	6.22	116.34	110.30
1	A	715	ILE	N-CA-C	6.15	117.10	111.81
1	A	534	PRO	CA-C-N	6.14	126.70	120.38
1	A	534	PRO	C-N-CA	6.14	126.70	120.38
1	A	1039	ASP	N-CA-C	5.99	117.95	108.79
1	A	384	GLU	N-CA-C	5.96	118.90	110.50
1	A	1013	THR	N-CA-C	-5.90	105.40	113.30
1	A	690	ILE	N-CA-C	5.80	116.16	107.51
1	A	723	ILE	N-CA-C	5.76	113.76	107.60
3	C	109	DA	C2'-C3'-O3'	-5.74	102.89	111.50
1	A	464	LEU	N-CA-C	5.65	118.20	110.01
1	A	571	ASP	N-CA-C	-5.58	106.36	112.72
1	A	1115	ARG	N-CA-C	5.55	117.14	111.14
1	A	524	ASP	N-CA-C	5.52	119.11	112.93
1	A	855	PHE	N-CA-C	5.50	118.00	110.24
1	A	433	LYS	CA-C-N	-5.50	113.92	120.13
1	A	433	LYS	C-N-CA	-5.50	113.92	120.13
1	A	1064	SER	N-CA-C	-5.45	100.41	109.46
1	A	574	ALA	CA-C-N	-5.32	114.86	120.66
1	A	574	ALA	C-N-CA	-5.32	114.86	120.66
1	A	751	PHE	N-CA-C	-5.32	104.39	112.04
1	A	767	GLN	N-CA-C	5.28	117.44	111.11
1	A	1146	TYR	N-CA-C	5.12	116.12	109.72
1	A	755	ILE	CB-CA-C	-5.11	105.17	112.22
1	A	1050	LEU	N-CA-C	5.10	116.69	111.03
1	A	532	VAL	N-CA-C	5.08	115.17	107.75
1	A	635	VAL	N-CA-C	5.05	116.81	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	609	VAL	N-CA-C	5.04	115.11	107.75
1	A	796	PHE	N-CA-C	5.03	117.65	111.82
1	A	1127	SER	N-CA-C	-5.03	107.19	113.72
1	A	527	ASN	N-CA-C	5.01	117.23	108.76
1	A	940	LEU	N-CA-C	-5.01	105.90	111.36
3	C	121	DC	C2'-C3'-O3'	-5.00	104.00	111.50

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 ⓘ

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	626	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	663	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 44.

All (663) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:908:MET:HE1	1:A:916:ARG:HD2	1.51	0.91
3:C:115:DT:H2''	3:C:116:DC:C5'	2.01	0.91
1:A:1074:LEU:O	1:A:1075:LYS:HD3	1.71	0.91
1:A:636:GLY:C	1:A:639:ILE:HD11	1.97	0.89
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: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:990:MET:HE1	1:A:1032:LEU:HD11	1.57	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:727:ASN:HD22	1:A:727:ASN:N	1.77	0.83
1:A:1007:MET:HE2	1:A:1044:PHE:HE2	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:662:ILE:HG23	1:A:663:GLY:N	2.02	0.75
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:962:PHE:CZ	1:A:964:TYR:HB2	2.25	0.72
1:A:545:LYS:HZ3	1:A:745:THR:HG23	1.55	0.71
1:A:548:GLN:H	1:A:725:MET:HE1	1.54	0.71
1:A:710:GLU:H	1:A:710:GLU:CD	1.98	0.71
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:548:GLN:H	1:A:725:MET:CE	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1130:VAL:O	1:A:1134:GLU:HG2	1.95	0.67
1:A:438:ASN:OD1	1:A:449:LYS:HG3	1.95	0.66
1:A:540:MET:HE2	1:A:634:ILE:HG12	1.78	0.66
1:A:621:PHE:O	1:A:625:LYS:HG2	1.94	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:1007:MET:HE2	1:A:1044:PHE:CE2	2.29	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:505:GLN:HB2	1:A:519:MET:HE3	1.78	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:583:PHE:CD1	1:A:583:PHE:C	2.74	0.64
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:1113:GLN:HE21	1:A:1238:TRP:NE1	1.96	0.64
1:A:410:MET:HE2	1:A:410:MET:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:660:SER:C	1:A:662:ILE:H	2.05	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: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
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:569:ALA:C	1:A:570:LEU:HD23	2.25	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:430:PHE:C	1:A:430:PHE:CD1	2.79	0.61
1:A:585:VAL:HG22	1:A:618:LEU:HD12	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:6:DG:H2''	2:B:7:DA:C5'	2.31	0.60
1:A:395:LYS:C	1:A:396:ILE:HD12	2.26	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: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: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
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:386:THR:C	1:A:387:LEU:HD23	2.28	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:669:ASN:N	1:A:669:ASN:ND2	2.44	0.58
1:A:664:ARG:HD2	1:A:687:GLY:C	2.28	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:660:SER:C	1:A:662:ILE:N	2.62	0.58
1:A:1002:ASP:O	1:A:1003:THR:HB	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:583:PHE:C	1:A:583:PHE:HD1	2.12	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:1181:GLN:HA	1:A:1181:GLN:NE2	2.09	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
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:697:ALA:C	1:A:699:GLU:N	2.61	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:544:MET:HE3	1:A:647:LEU:HD13	1.88	0.56
1:A:908:MET:CE	1:A:916:ARG:HD2	2.29	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:558:ILE:C	1:A:558:ILE:HD12	2.31	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:962:PHE:CD1	1:A:962:PHE:C	2.82	0.56
1:A:1184:SER:C	1:A:1185:ASN:HD22	2.13	0.55
1:A:859:LEU:CB	1:A:1038:ILE:HD11	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1129:PRO:C	1:A:1131:SER:N	2.64	0.55
1:A:344:TYR:CE2	1:A:535:PRO:HD3	2.42	0.55
1:A:654:CYS:O	1:A:655:LYS:C	2.49	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: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:990:MET:HG2	1:A:994:MET:CE	2.38	0.54
1:A:553:HIS:O	1:A:554:GLN:HG3	2.08	0.54
1:A:896:GLU:C	1:A:896:GLU:CD	2.76	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:797:TYR:O	1:A:798:GLU:C	2.51	0.53
1:A:940:LEU:O	1:A:944:ILE:HG13	2.09	0.53
1:A:544:MET:HE1	1:A:557:ILE:HD13	1.90	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:710:GLU:CD	1:A:710:GLU:N	2.66	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:872:PHE:HD1	1:A:901:LEU:HD13	1.74	0.53
1:A:1160:TRP:NE1	1:A:1197:GLN:HE22	2.06	0.53
1:A:1087:LEU:HG	1:A:1216:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:908:MET:HE1	1:A:916:ARG:CD	2.31	0.53
1:A:957:TYR:O	1:A:960:LEU:HB2	2.08	0.53
1:A:1086:ASP:O	1:A:1087:LEU:C	2.51	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:505:GLN:HB2	1:A:519:MET:CE	2.39	0.52
1:A:731:MET:HA	1:A:737:GLN:CB	2.40	0.52
1:A:791:LEU:HD23	1:A:956:MET:HE1	1.90	0.52
1:A:351:ASP:C	1:A:353:TYR:H	2.18	0.52
1:A:697:ALA:C	1:A:699:GLU:H	2.18	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: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: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
2:B:6:DG:H2''	2:B:7:DA:H5''	1.91	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:545:LYS:HZ3	1:A:745:THR:CG2	2.23	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:495:GLY:O	1:A:496:PRO:C	2.53	0.51
1:A:505:GLN:CB	1:A:519:MET:HE3	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:596:TYR:O	1:A:597:ALA:HB3	2.09	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: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:H	2.18	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:363:GLY:C	1:A:364:LYS:HG2	2.35	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:594:PHE:O	1:A:595:PRO:C	2.55	0.50
1:A:1014:ASN:C	1:A:1014:ASN:HD22	2.19	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:C	1:A:667:ARG:HG3	2.36	0.49
1:A:568:PHE:CE2	1:A:575:PRO:CD	2.96	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:718:THR:HG22	1:A:719:GLU:N	2.26	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:1236:ALA:O	1:A:1237:THR:C	2.55	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:1086:ASP:O	1:A:1088:ALA:N	2.46	0.49
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:935:ASN:C	1:A:935:ASN:HD22	2.20	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:1094:PHE:CD1	1:A:1094:PHE:C	2.91	0.48
1:A:660:SER:O	1:A:663:GLY:N	2.47	0.48
1:A:990:MET:HG2	1:A:994:MET:HE2	1.95	0.48
1:A:1154:HIS:CE1	1:A:1155:VAL:HG23	2.48	0.48
1:A:594:PHE:C	1:A:595:PRO:O	2.56	0.48
1:A:870:GLN:O	1:A:871:GLU:C	2.57	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:VAL:C	1:A:655:LYS:H	2.22	0.48
1:A:747:LYS:HZ2	1:A:750:LYS:HD3	1.78	0.48
1:A:568:PHE:CD2	1:A:575:PRO:CD	2.97	0.47
1:A:1243:PRO:O	1:A:1244:THR:C	2.57	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:767:GLN:O	1:A:768:ILE:C	2.57	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: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:1215:GLN:C	1:A:1218:PRO:HD2	2.40	0.47
1:A:548:GLN:HB2	1:A:725:MET:HE1	1.97	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:1085:CYS:O	1:A:1086:ASP:C	2.56	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: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:440:ALA:C	1:A:441:PHE:CG	2.94	0.46
1:A:926:LYS:HD2	1:A:946:GLN:OE1	2.15	0.46
1:A:941:GLN:OE1	1:A:944:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1010:THR:C	1:A:1012:SER:H	2.22	0.46
1:A:395:LYS:CA	1:A:408:ILE:HD11	2.46	0.46
1:A:992:GLN:C	1:A:994:MET:H	2.24	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: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:849:VAL:HA	1:A:1049:LEU:O	2.15	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:697:ALA:O	1:A:698:LYS:C	2.56	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:548:GLN:CB	1:A:725:MET:HE1	2.46	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: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
1:A:1029:VAL:O	1:A:1030:ASN:C	2.60	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:1010:THR:C	1:A:1012:SER:N	2.75	0.45
1:A:556:GLU:HA	1:A:615:GLU:OE2	2.17	0.45
1:A:587:SER:OG	1:A:614:THR:O	2.35	0.45
1:A:1179:ILE:HG22	1:A:1207:ASP:HB2	1.99	0.45
1:A:494:LYS:C	1:A:773:GLY:HA2	2.41	0.44
1:A:911:LEU:O	1:A:914:GLU:HB2	2.17	0.44
1:A:1116:LEU:O	1:A:1117:ILE:C	2.59	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:565:HIS:CE1	1:A:580:GLN:CD	2.94	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:1242:ASP:OD1	1:A:1244:THR:OG1	2.26	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:992:GLN:C	1:A:994:MET:N	2.74	0.44
1:A:861:PHE:HA	1:A:1038:ILE:HA	2.00	0.44
1:A:991:VAL:HA	1:A:994:MET:HE3	2.00	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:731:MET:HE2	1:A:737:GLN:O	2.17	0.44
1:A:1133:PHE:O	1:A:1134:GLU:C	2.61	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: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:699:GLU:CG	1:A:784:ARG:HH22	2.31	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:950:LYS:O	1:A:951:LEU:C	2.61	0.43
1:A:1014:ASN:C	1:A:1014:ASN:ND2	2.76	0.43
1:A:1053:LYS:CD	2:B:10:DG:H1'	2.42	0.43
1:A:1182:ASP:CG	1:A:1193:TYR:HH	2.25	0.43
1:A:1224:CYS:O	1:A:1225:GLU:C	2.62	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:548:GLN:H	1:A:725:MET:HE3	1.84	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:1090:ASP:O	1:A:1091:THR:C	2.62	0.43
1:A:545:LYS:HZ3	1:A:745:THR:CB	2.32	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:638:ASN:O	1:A:638:ASN:CG	2.62	0.42
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:1108:ILE:O	1:A:1109:VAL:C	2.62	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:789:GLU:CD	1:A:966:ARG:HD2	2.44	0.42
1:A:840:ALA:C	1:A:981:ARG:HH12	2.28	0.42
1:A:370:ALA:O	1:A:371:GLU:C	2.61	0.42
1:A:494:LYS:HA	1:A:773:GLY:CA	2.50	0.42
3:C:120:DG:H2''	3:C:121:DC:OP2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:563:LEU:HB3	1:A:579:PHE:CB	2.49	0.42
1:A:725:MET:HB3	1:A:725:MET:HE2	1.59	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: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:843:LEU:HD12	1:A:843:LEU:C	2.44	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:1185:ASN:ND2	1:A:1185:ASN:C	2.78	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:652:ASN:HB2	1:A:670:MET:CE	2.50	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:1055:TYR:CD1	1:A:1055:TYR:C	2.98	0.41
1:A:1127:SER:O	1:A:1129:PRO:HD3	2.20	0.41
1:A:1166:GLY:O	1:A:1167:ARG:C	2.63	0.41
1:A:338:GLU:O	1:A:339:GLN:HB2	2.19	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:514:CYS:O	1:A:515:LYS:C	2.63	0.41
1:A:645:GLU:HG3	1:A:649:GLN:CD	2.45	0.41
1:A:945:ARG:HG2	1:A:949:LEU:HD12	2.03	0.41
1:A:708:LEU:HD23	1:A:720:ARG:NE	2.36	0.41
1:A:351:ASP:C	1:A:353:TYR:N	2.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:375:SER:OG	1:A:630:ASP:OD2	2.30	0.41
1:A:493:ILE:HG12	1:A:528:VAL:CG2	2.51	0.41
1:A:776:MET:O	1:A:777:SER:C	2.64	0.41
1:A:797:TYR:C	1:A:799:ASN:N	2.78	0.41
1:A:865:TYR:OH	1:A:977:THR:HG22	2.20	0.41
1:A:637:HIS:O	1:A:638:ASN:C	2.64	0.41
1:A:652:ASN:HD22	1:A:670:MET:HE3	1.84	0.41
1:A:903:ASP:C	1:A:905:SER:H	2.28	0.41
1:A:1074:LEU:C	1:A:1075:LYS:HD3	2.43	0.41
1:A:548:GLN:NE2	1:A:554:GLN:O	2.54	0.41
1:A:558:ILE:C	1:A:558:ILE:CD1	2.94	0.41
1:A:696:SER:CB	1:A:761:VAL:HG11	2.51	0.41
1:A:727:ASN:N	1:A:727:ASN:ND2	2.47	0.41
1:A:864:LEU:O	1:A:868:ILE:HG13	2.21	0.41
1:A:865:TYR:O	1:A:866:PRO:C	2.63	0.41
1:A:984:LEU:O	1:A:984:LEU:HG	2.21	0.41
1:A:1022:GLY:C	1:A:1024:LYS:N	2.75	0.41
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:925:VAL:C	1:A:927:GLN:N	2.77	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:652:ASN:ND2	1:A:670:MET:HE3	2.36	0.40
1:A:922:ARG:NH1	1:A:950:LYS:CB	2.82	0.40
1:A:1099:ILE:C	1:A:1101:SER:N	2.78	0.40
1:A:1148:ASP:OD1	1:A:1148:ASP:O	2.39	0.40
1:A:1185:ASN:HD22	1:A:1185:ASN:C	2.29	0.40
1:A:408:ILE:CG2	1:A:409:SER:N	2.82	0.40
1:A:640:TYR:CE1	1:A:781:MET:HE3	2.56	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:903:ASP:C	1:A:905:SER:N	2.79	0.40
1:A:1125:ASN:OD1	1:A:1125:ASN:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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

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%)	3 7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	GLN
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	717 (92%)	66 (8%)	10	26

All (66) 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	500	GLU
1	A	535	PRO
1	A	539	VAL
1	A	555	ASN
1	A	570	LEU

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Mol	Chain	Res	Type
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	609	VAL
1	A	610	GLU
1	A	614	THR
1	A	619	LEU
1	A	634	ILE
1	A	651	ILE
1	A	669	ASN
1	A	685	THR
1	A	686	CYS
1	A	695	ILE
1	A	721	VAL
1	A	727	ASN
1	A	729	GLN
1	A	730	ASN
1	A	735	SER
1	A	738	LEU
1	A	755	ILE
1	A	757	CYS
1	A	759	LEU
1	A	764	LEU
1	A	779	THR
1	A	802	ILE
1	A	846	ASP
1	A	880	GLN
1	A	896	GLU
1	A	937	ASP
1	A	946	GLN
1	A	956	MET
1	A	1007	MET
1	A	1011	ASN
1	A	1039	ASP
1	A	1053	LYS
1	A	1077	LEU
1	A	1080	VAL
1	A	1102	ASP

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Mol	Chain	Res	Type
1	A	1108	ILE
1	A	1131	SER
1	A	1134	GLU
1	A	1149	LYS
1	A	1156	HIS
1	A	1178	VAL
1	A	1179	ILE
1	A	1181	GLN
1	A	1185	ASN
1	A	1199	GLN
1	A	1242	ASP
1	A	1247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) 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	566	HIS
1	A	669	ASN
1	A	683	ASN
1	A	727	ASN
1	A	729	GLN
1	A	730	ASN
1	A	737	GLN
1	A	760	ASN
1	A	767	GLN
1	A	770	ASN
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
1	A	1011	ASN
1	A	1014	ASN
1	A	1023	ASN

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Mol	Chain	Res	Type
1	A	1072	GLN
1	A	1098	GLN
1	A	1111	ASN
1	A	1113	GLN
1	A	1122	ASN
1	A	1132	GLN
1	A	1144	GLN
1	A	1154	HIS
1	A	1181	GLN
1	A	1185	ASN
1	A	1197	GLN
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 oligosaccharides 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	28,29,29	2.57	6 (21%)	41,45,45	0.83	1 (2%)

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	-	4/22/34/34	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	DCP	PB-O3A	7.21	1.67	1.59
4	A	1301	DCP	PB-O3B	6.54	1.66	1.59
4	A	1301	DCP	PA-O3A	5.86	1.65	1.59
4	A	1301	DCP	PG-O1G	3.28	1.60	1.50
4	A	1301	DCP	PB-O1B	3.10	1.61	1.50
4	A	1301	DCP	C4-N4	2.13	1.39	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DCP	O4'-C1'-N1	2.09	111.58	107.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

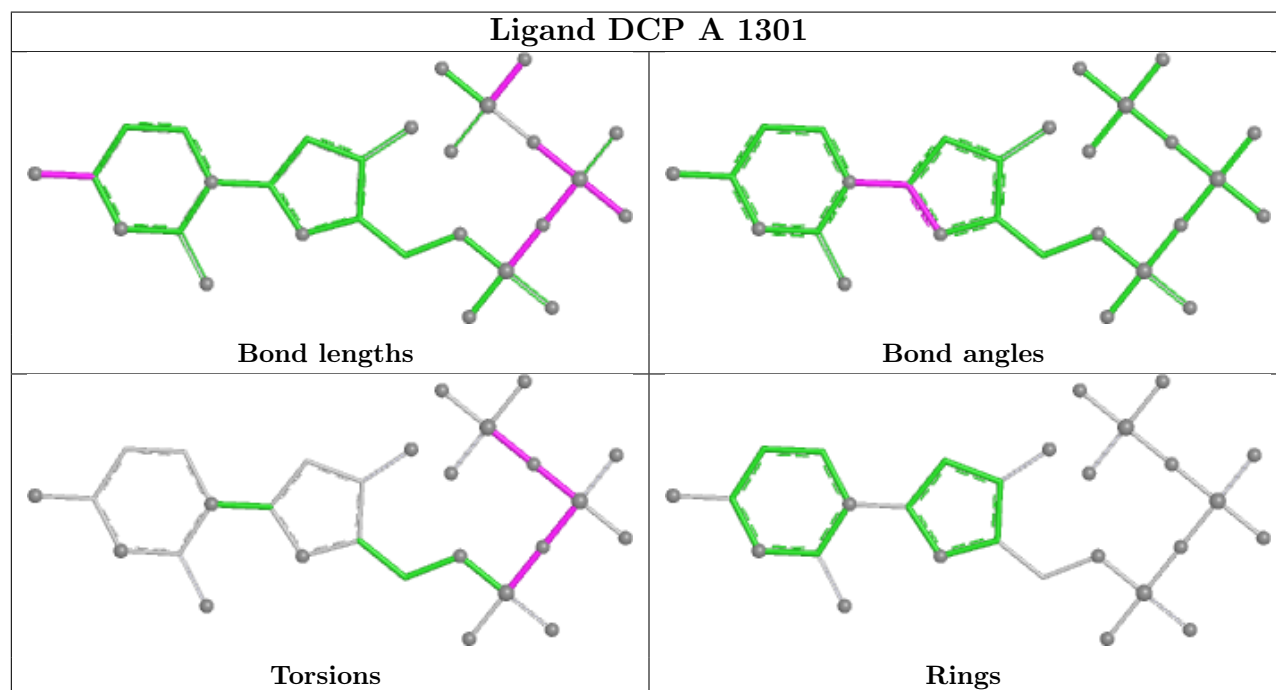
Mol	Chain	Res	Type	Atoms
4	A	1301	DCP	PB-O3B-PG-O3G
4	A	1301	DCP	PB-O3A-PA-O2A
4	A	1301	DCP	PA-O3A-PB-O2B
4	A	1301	DCP	PG-O3B-PB-O2B

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	870/922 (94%)	0.79	141 (16%) 4 4	7, 52, 113, 138	0
2	B	11/11 (100%)	0.14	0 100 100	26, 43, 66, 68	0
3	C	13/13 (100%)	0.37	1 (7%) 19 17	22, 41, 72, 86	0
All	All	894/946 (94%)	0.78	142 (15%) 5 4	7, 52, 112, 138	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	725	MET	6.4
1	A	882	VAL	5.0
1	A	696	SER	4.6
1	A	732	TYR	4.5
1	A	1152	LEU	4.3
1	A	597	ALA	4.2
1	A	1203	ASN	4.2
1	A	724	PRO	4.0
1	A	596	TYR	4.0
1	A	646	VAL	3.9
1	A	735	SER	3.9
1	A	1140	THR	3.9
1	A	682	ARG	3.9
1	A	734	GLU	3.8
1	A	719	GLU	3.8
1	A	553	HIS	3.7
1	A	934	LEU	3.7
1	A	401	GLY	3.7
1	A	1173	ASP	3.7
1	A	1066	GLY	3.7
1	A	1151	SER	3.6
1	A	1146	TYR	3.6
1	A	706	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1149	LYS	3.5
1	A	1158	ALA	3.5
1	A	673	LEU	3.5
1	A	1198	LEU	3.5
1	A	1171	ALA	3.5
1	A	1195	PRO	3.4
1	A	1172	GLY	3.4
1	A	398	LEU	3.4
1	A	396	ILE	3.4
1	A	551	LYS	3.3
1	A	607	VAL	3.3
1	A	1150	LYS	3.3
1	A	554	GLN	3.2
1	A	678	GLY	3.2
1	A	636	GLY	3.2
1	A	681	GLU	3.2
1	A	1212	LEU	3.2
1	A	680	GLY	3.1
1	A	697	ALA	3.1
1	A	1169	VAL	3.1
1	A	1167	ARG	3.1
1	A	550	ALA	3.1
1	A	704	LYS	3.1
1	A	1205	THR	3.0
1	A	1148	ASP	3.0
1	A	703	CYS	3.0
1	A	933	ASP	3.0
1	A	547	MET	3.0
1	A	1154	HIS	3.0
1	A	1165	GLY	3.0
1	A	1141	LYS	2.9
1	A	1193	TYR	2.9
1	A	727	ASN	2.9
1	A	601	VAL	2.9
1	A	407	PRO	2.9
1	A	589	PRO	2.9
1	A	1204	LEU	2.8
1	A	403	GLU	2.8
1	A	705	SER	2.8
1	A	442	GLU	2.8
1	A	622	PHE	2.8
1	A	546	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	668	SER	2.8
1	A	736	SER	2.8
1	A	605	LYS	2.8
1	A	399	ASN	2.8
1	A	746	TRP	2.7
1	A	640	TYR	2.7
1	A	1139	LEU	2.7
1	A	1157	VAL	2.7
1	A	394	MET	2.7
1	A	671	PRO	2.7
1	A	1199	GLN	2.7
1	A	670	MET	2.7
1	A	593	ILE	2.6
1	A	728	ILE	2.6
1	A	1189	SER	2.6
1	A	1168	LYS	2.6
1	A	644	LEU	2.6
1	A	1196	GLU	2.6
1	A	1147	PRO	2.5
1	A	740	TYR	2.5
1	A	700	LEU	2.5
1	A	1130	VAL	2.5
1	A	701	ILE	2.5
1	A	723	ILE	2.5
1	A	738	LEU	2.5
1	A	557	ILE	2.5
1	A	709	SER	2.5
1	A	684	ALA	2.4
1	A	1200	LYS	2.4
1	A	566	HIS	2.4
1	A	742	LEU	2.4
1	A	938	LEU	2.4
1	A	753	LEU	2.4
1	A	745	THR	2.4
1	A	679	PHE	2.3
1	A	602	ILE	2.3
1	A	1161	ILE	2.3
1	A	672	LYS	2.3
1	A	937	ASP	2.3
1	A	749	ALA	2.3
1	A	741	LEU	2.3
1	A	637	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	558	ILE	2.3
1	A	685	THR	2.3
1	A	834	ARG	2.3
1	A	555	ASN	2.3
1	A	556	GLU	2.3
1	A	1138	ALA	2.3
1	A	575	PRO	2.3
1	A	936	PRO	2.3
1	A	925	VAL	2.2
1	A	1143	PRO	2.2
1	A	932	GLN	2.2
1	A	590	LYS	2.2
1	A	935	ASN	2.2
3	C	109	DA	2.2
1	A	1016	GLU	2.2
1	A	406	THR	2.2
1	A	716	LEU	2.2
1	A	1153	PRO	2.1
1	A	571	ASP	2.1
1	A	1065	ASP	2.1
1	A	1166	GLY	2.1
1	A	835	LYS	2.1
1	A	757	CYS	2.1
1	A	586	VAL	2.1
1	A	722	VAL	2.1
1	A	657	PRO	2.1
1	A	470	GLY	2.1
1	A	650	ARG	2.1
1	A	472	THR	2.1
1	A	699	GLU	2.1
1	A	549	ASN	2.0
1	A	594	PHE	2.0
1	A	944	ILE	2.0
1	A	1188	ALA	2.0
1	A	1208	THR	2.0

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

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

6.3 Carbohydrates [i](#)

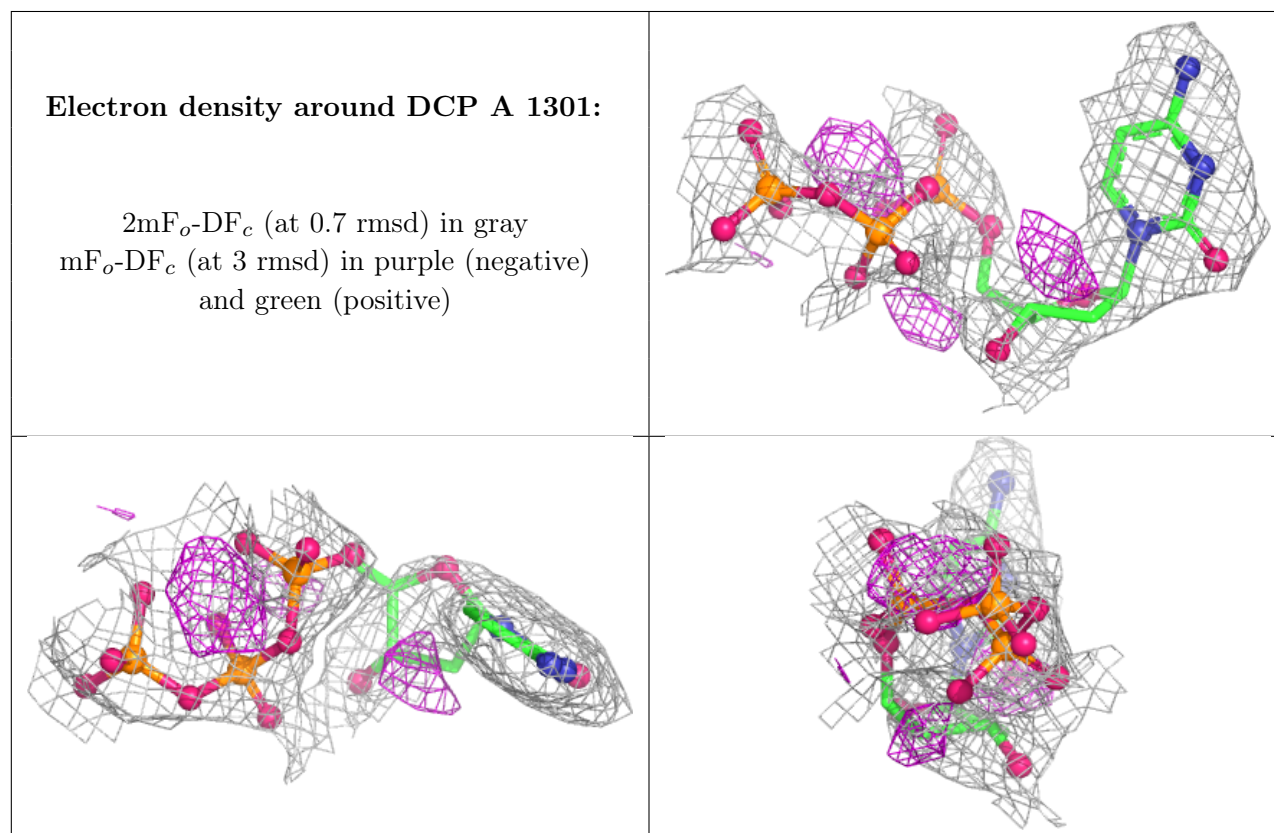
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DCP	A	1301	28/28	0.83	0.16	42,85,136,136	0
5	MG	A	1302	1/1	0.95	0.10	44,44,44,44	0
6	CO	C	401	1/1	0.95	0.15	73,73,73,73	0
5	MG	A	1303	1/1	0.96	0.09	51,51,51,51	0
6	CO	B	101	1/1	0.97	0.13	62,62,62,62	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.