



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 03:05 am BST

PDB ID : 6I8A
Title : The crystal structure of the Pol2 catalytic domain of DNA polymerase epsilon carrying a P301R substitution.
Authors : Parkash, V.; Johansson, E.
Deposited on : 2018-11-19
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

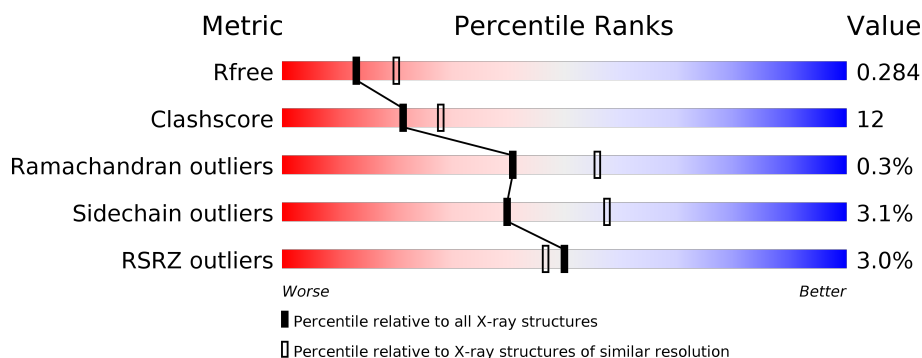
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 on 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	1190	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>21%</div> <div>• 7%</div> </div> </div>
1	B	1190	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>• 8%</div> </div> </div>
2	C	11	<div> <div>45%</div> <div>55%</div> </div>
2	P	11	<div> <div>73%</div> <div>27%</div> </div>
3	D	16	<div> <div>63%</div> <div>31%</div> <div>6%</div> </div>
3	T	16	<div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18065 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 epsilon catalytic subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1107	Total	C	N	O	S	0	0	0
			8569	5509	1417	1600	43			
1	B	1094	Total	C	N	O	S	0	0	0
			8369	5372	1388	1568	41			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P21951
A	-3	GLY	-	expression tag	UNP P21951
A	-2	ASP	-	expression tag	UNP P21951
A	-1	PRO	-	expression tag	UNP P21951
A	0	HIS	-	expression tag	UNP P21951
A	301	ARG	PRO	engineered mutation	UNP P21951
B	-4	GLY	-	expression tag	UNP P21951
B	-3	GLY	-	expression tag	UNP P21951
B	-2	ASP	-	expression tag	UNP P21951
B	-1	PRO	-	expression tag	UNP P21951
B	0	HIS	-	expression tag	UNP P21951
B	301	ARG	PRO	engineered mutation	UNP P21951

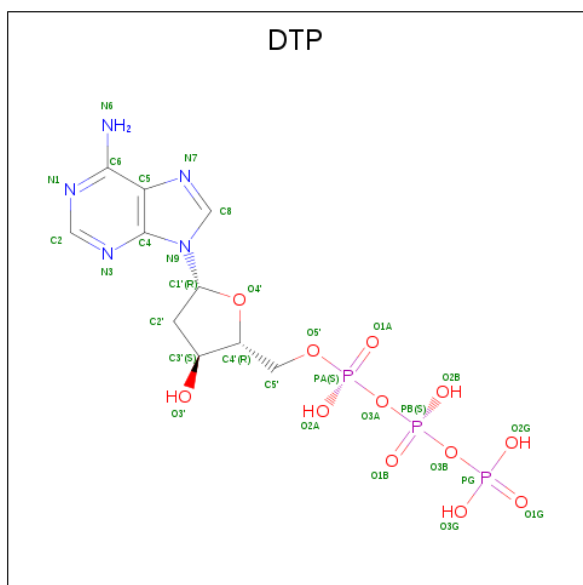
- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	4	0	0
			220	105	38	66	11			
2	C	11	Total	C	N	O	P	4	0	0
			220	105	38	66	11			

- Molecule 3 is a DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	15	Total	C	N	O	P	0	0	0
			308	147	54	92	15			
3	D	15	Total	C	N	O	P	0	0	0
			307	146	54	92	15			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (three-letter code: DTP) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		
4	B	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 6 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	Fe 1	0	0

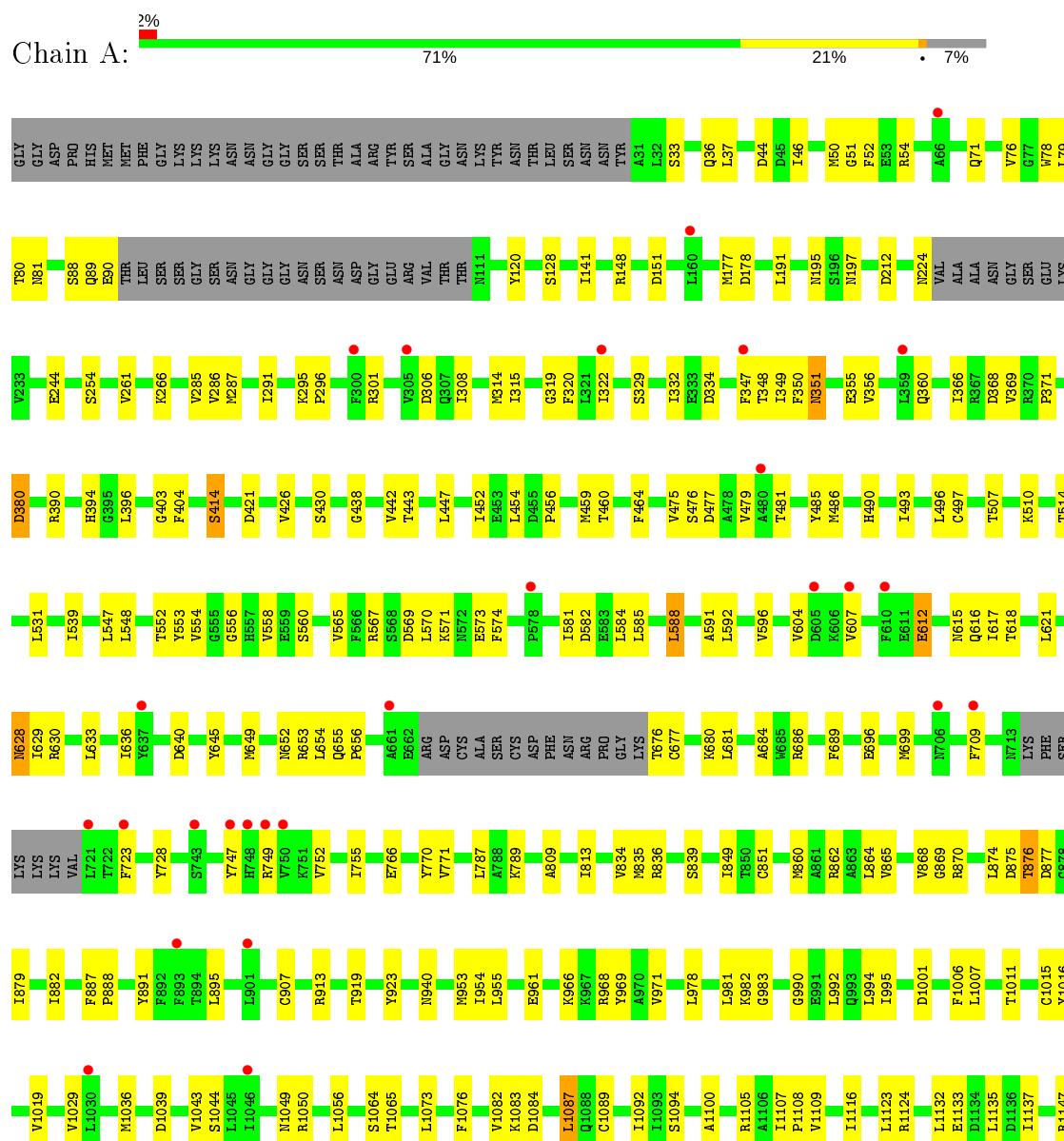
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total 2	O 2	0	0
7	T	1	Total 1	O 1	0	0
7	B	3	Total 3	O 3	0	0

3 Residue-property plots

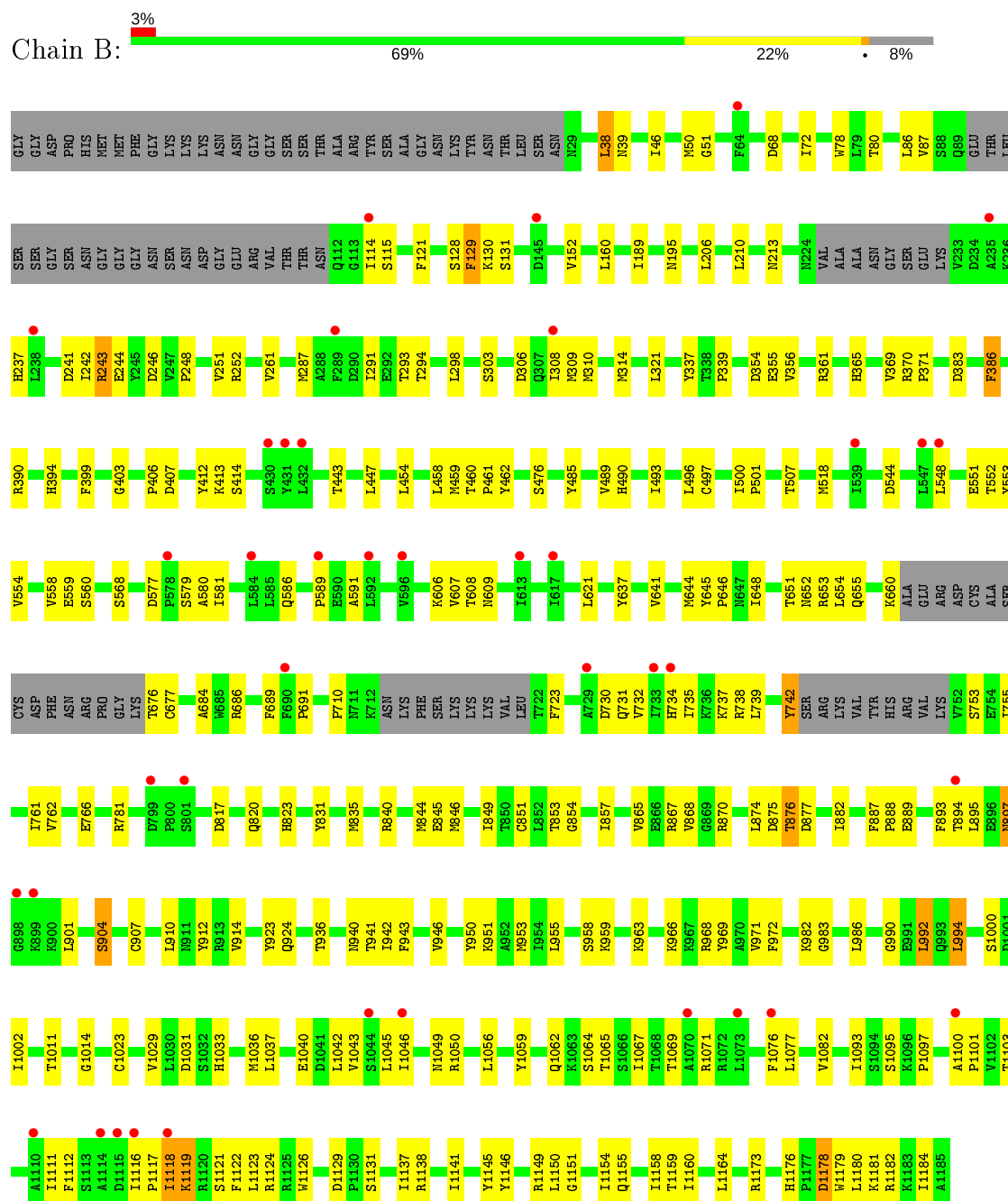
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

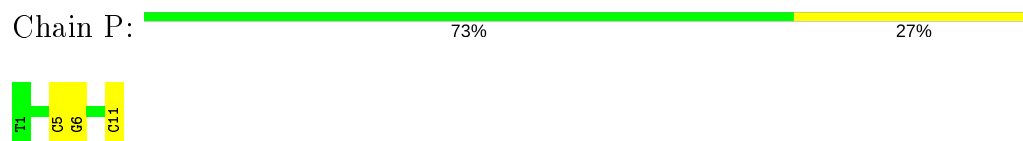




- Molecule 1: DNA polymerase epsilon catalytic subunit A



- Molecule 2: Primer DNA



- Molecule 2: Primer DNA

Chain C:  45% 55%



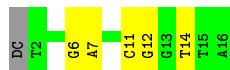
- Molecule 3: Template DNA

Chain T:  75% 19% 6%



- Molecule 3: Template DNA

Chain D:  63% 31% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	154.47Å 70.26Å 159.34Å 90.00° 112.85° 90.00°	Depositor
Resolution (Å)	19.96 – 2.65 48.94 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.96-2.65) 98.9 (48.94-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.65Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.229 , 0.279 0.238 , 0.284	Depositor DCC
R_{free} test set	4588 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18065	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.15 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3325e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: DOC, CA, DTP, FE

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	0.35	0/8768	0.51	0/11921
1	B	0.37	0/8563	0.54	0/11657
2	C	0.82	0/225	1.05	0/344
2	P	0.82	0/225	0.96	0/344
3	D	0.79	0/343	0.95	0/527
3	T	0.74	0/344	1.00	0/529
All	All	0.40	0/18468	0.57	0/25322

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8569	0	8038	176	0
1	B	8369	0	7767	224	0
2	C	220	0	122	8	0
2	P	220	0	122	2	0
3	D	307	0	168	4	0
3	T	308	0	171	2	0
4	A	30	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	12	0	0
5	A	2	0	0	1	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	2	0	0	0	0
7	B	3	0	0	0	0
7	T	1	0	0	0	0
All	All	18065	0	16412	408	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 12.

All (408) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1076:PHE:HE1	1:B:1118:ILE:CD1	1.52	1.23
1:B:1076:PHE:HE1	1:B:1118:ILE:HD12	1.07	1.10
1:B:1137:ILE:O	1:B:1141:ILE:HG12	1.54	1.06
1:B:1076:PHE:CE1	1:B:1118:ILE:HD12	1.90	1.05
1:B:454:LEU:CD1	1:B:459:MET:HG3	1.88	1.02
1:B:454:LEU:HD12	1:B:459:MET:HG3	1.39	1.01
1:B:1112:PHE:CG	1:B:1137:ILE:HD11	1.97	1.00
1:B:1076:PHE:CE1	1:B:1118:ILE:CD1	2.44	0.98
1:B:641:VAL:HG21	1:B:644:MET:HG3	1.46	0.95
1:B:454:LEU:HD12	1:B:459:MET:CG	1.97	0.94
1:B:644:MET:HE1	1:B:854:GLY:CA	1.99	0.92
1:B:1138:ARG:HH21	1:B:1138:ARG:HG3	1.39	0.87
1:B:691:PRO:HG2	1:B:742:TYR:HE1	1.39	0.87
1:A:567:ARG:HB2	1:A:570:LEU:HD13	1.57	0.87
1:B:644:MET:HE1	1:B:854:GLY:HA3	1.57	0.87
1:A:332:ILE:HG22	1:A:351:ASN:HD21	1.43	0.84
1:B:454:LEU:CD1	1:B:459:MET:CG	2.54	0.83
1:A:655:GLN:HG2	1:A:770:TYR:HB3	1.61	0.82
1:B:51:GLY:O	1:B:128:SER:HB2	1.80	0.82
1:B:644:MET:CE	1:B:854:GLY:CA	2.57	0.81
1:B:644:MET:CE	1:B:854:GLY:HA3	2.12	0.79
1:B:1119:LYS:HB2	1:B:1119:LYS:NZ	1.96	0.79
1:B:994:LEU:HD21	1:B:1150:LEU:HD12	1.65	0.79
1:B:986:LEU:HD11	1:B:1000:SER:HB2	1.65	0.77
1:B:1112:PHE:CD2	1:B:1137:ILE:HD11	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:ARG:NH2	1:B:1138:ARG:HG3	1.98	0.76
1:A:953:MET:HG3	1:A:971:VAL:HG22	1.69	0.73
1:B:644:MET:CE	1:B:854:GLY:HA2	2.18	0.73
1:B:870:ARG:HD3	1:B:882:ILE:HD11	1.71	0.72
1:B:655:GLN:HA	1:B:846:MET:HE2	1.68	0.72
1:B:1116:ILE:HB	1:B:1117:PRO:HD3	1.69	0.72
1:B:1076:PHE:HE1	1:B:1118:ILE:HD11	1.51	0.72
1:B:955:LEU:HD23	1:B:969:TYR:HB3	1.70	0.72
1:A:653:ARG:NH1	1:A:766:GLU:O	2.23	0.71
1:A:868:VAL:CG2	1:A:887:PHE:HE1	2.04	0.71
1:B:1119:LYS:HG2	1:B:1123:LEU:HD12	1.72	0.71
1:B:644:MET:HE3	1:B:648:ILE:HD11	1.72	0.70
1:A:286:VAL:HG11	1:A:486:MET:SD	2.33	0.69
1:B:310:MET:HB2	1:B:321:LEU:HD21	1.72	0.69
1:B:1093:ILE:HD11	1:B:1145:TYR:CD1	2.28	0.69
1:B:607:VAL:HG21	1:B:893:PHE:HB3	1.74	0.69
1:B:653:ARG:NH1	1:B:766:GLU:O	2.25	0.69
1:B:553:TYR:HE1	1:B:835:MET:SD	2.15	0.69
1:A:870:ARG:HB2	1:A:882:ILE:HG22	1.74	0.68
1:B:580:ALA:HA	1:B:867:ARG:HH21	1.58	0.68
1:B:1076:PHE:CE1	1:B:1118:ILE:HD11	2.27	0.68
1:B:46:ILE:HD13	1:B:403:GLY:HA2	1.76	0.68
1:B:676:THR:HG23	1:B:677:CYS:H	1.57	0.68
1:A:360:GLN:HE21	1:A:396:LEU:HD21	1.60	0.67
1:B:651:THR:HG22	1:B:940:ASN:HA	1.77	0.67
1:B:1011:THR:HG23	1:B:1014:GLY:H	1.59	0.66
1:B:1031:ASP:OD2	1:B:1173:ARG:NH1	2.29	0.66
1:A:865:VAL:HA	1:A:868:VAL:HG12	1.78	0.65
1:A:553:TYR:HE2	1:A:851:CYS:HG	1.42	0.65
1:B:369:VAL:HG23	1:B:371:PRO:HD3	1.79	0.65
1:A:553:TYR:HE1	1:A:835:MET:SD	2.19	0.64
1:A:612:GLU:O	1:A:616:GLN:HG3	1.97	0.64
1:B:853:THR:O	1:B:857:ILE:HG12	1.98	0.64
1:A:574:PHE:HE2	1:A:882:ILE:HG23	1.63	0.64
1:B:87:VAL:HG23	1:B:114:ILE:HB	1.78	0.64
1:B:691:PRO:CG	1:B:742:TYR:HE1	2.11	0.64
1:A:315:ILE:HG21	1:A:369:VAL:HG11	1.80	0.64
1:B:210:LEU:HD11	1:B:242:ILE:HG23	1.80	0.64
1:B:1112:PHE:CD1	1:B:1137:ILE:HD11	2.32	0.63
1:B:1046:ILE:HG23	1:B:1146:TYR:CE2	2.32	0.63
1:B:454:LEU:HD11	1:B:459:MET:HG3	1.76	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:SER:HB2	1:B:195:ASN:HA	1.81	0.63
1:A:1056:LEU:HB2	1:A:1082:VAL:HG21	1.80	0.63
1:A:585:LEU:HA	1:A:588:LEU:CD2	2.30	0.62
1:A:584:LEU:O	1:A:588:LEU:HD23	2.00	0.62
1:B:641:VAL:CG2	1:B:644:MET:HG3	2.25	0.62
1:A:656:PRO:HG3	1:A:834:VAL:HG22	1.82	0.62
1:A:868:VAL:HG22	1:A:887:PHE:HE1	1.65	0.61
1:A:640:ASP:OD1	5:A:1302:CA:CA	1.78	0.61
1:B:337:TYR:CZ	1:B:339:PRO:HG3	2.35	0.61
1:A:681:LEU:HB2	1:A:849:ILE:HD13	1.82	0.61
1:B:986:LEU:CD1	1:B:1000:SER:HB2	2.31	0.61
1:B:1119:LYS:HG2	1:B:1123:LEU:CD1	2.30	0.61
1:B:121:PHE:CB	1:B:129:PHE:CE2	2.84	0.61
1:A:604:VAL:HA	1:A:607:VAL:HG22	1.83	0.60
1:B:1160:ILE:O	1:B:1164:LEU:HD12	2.00	0.60
1:B:1023:CYS:HB3	1:B:1154:ILE:HD13	1.83	0.60
1:A:452:ILE:HD12	1:A:476:SER:HB2	1.83	0.60
1:B:691:PRO:HG2	1:B:742:TYR:CE1	2.30	0.60
1:B:1103:THR:HG23	3:D:14:DT:OP1	2.03	0.59
1:B:1137:ILE:O	1:B:1141:ILE:CG1	2.41	0.59
1:B:968:ARG:HG2	1:B:983:GLY:HA3	1.84	0.59
1:B:50:MET:CE	1:B:370:ARG:HA	2.32	0.59
1:A:71:GLN:OE1	1:A:71:GLN:N	2.35	0.59
1:B:496:LEU:HG	1:B:500:ILE:HD12	1.83	0.59
1:B:454:LEU:HD11	1:B:459:MET:CG	2.29	0.58
1:B:553:TYR:HE2	1:B:851:CYS:HG	1.50	0.58
1:B:559:GLU:HA	1:B:966:LYS:HE2	1.84	0.58
1:B:653:ARG:NH2	1:B:924:GLN:O	2.37	0.58
1:A:567:ARG:NH1	1:A:1007:LEU:O	2.37	0.58
1:A:347:PHE:CE2	1:A:475:VAL:HG23	2.39	0.58
1:B:1037:LEU:HD23	1:B:1042:LEU:HD13	1.86	0.58
1:A:919:THR:HG23	1:A:940:ASN:HB2	1.86	0.57
1:A:148:ARG:HG3	1:A:151:ASP:OD1	2.03	0.57
1:A:50:MET:HA	1:A:50:MET:HE2	1.87	0.57
1:A:652:ASN:HB2	1:A:654:LEU:HG	1.86	0.57
1:A:322:ILE:HG22	1:A:350:PHE:HB2	1.86	0.57
1:B:1093:ILE:HD11	1:B:1145:TYR:CG	2.40	0.57
1:B:554:VAL:HG22	1:B:684:ALA:HB3	1.86	0.57
1:B:953:MET:HG3	1:B:971:VAL:HG22	1.86	0.57
1:B:1137:ILE:HG23	1:B:1141:ILE:HD11	1.86	0.57
1:A:1050:ARG:NH2	1:A:1065:THR:OG1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:VAL:HG12	1:A:394:HIS:CG	2.39	0.57
1:A:332:ILE:HG22	1:A:351:ASN:ND2	2.16	0.56
1:B:1056:LEU:HD11	1:B:1067:ILE:HG23	1.87	0.56
1:B:46:ILE:HD11	1:B:399:PHE:O	2.04	0.56
1:A:585:LEU:HA	1:A:588:LEU:HD23	1.86	0.56
1:A:314:MET:HG2	1:A:347:PHE:HZ	1.70	0.56
1:A:569:ASP:N	1:A:569:ASP:OD1	2.39	0.56
1:A:809:ALA:O	1:A:813:ILE:HG13	2.06	0.56
1:B:1154:ILE:HG22	1:B:1159:THR:HG23	1.87	0.56
1:B:731:GLN:O	1:B:735:ILE:HG13	2.05	0.56
1:B:1119:LYS:O	1:B:1123:LEU:HB2	2.07	0.55
1:B:865:VAL:HA	1:B:868:VAL:HG12	1.88	0.55
1:A:33:SER:O	1:A:37:LEU:HD12	2.07	0.55
1:B:1111:ILE:HD11	1:B:1122:PHE:HB2	1.88	0.55
1:B:644:MET:CE	1:B:648:ILE:HD11	2.36	0.55
1:B:1065:THR:O	1:B:1069:THR:HG23	2.07	0.55
1:A:573:GLU:O	1:A:870:ARG:NH1	2.40	0.54
1:B:686:ARG:HB2	1:B:755:ILE:HG12	1.89	0.54
1:A:1123:LEU:HD13	1:A:1135:LEU:HD12	1.90	0.54
1:A:868:VAL:HG22	1:A:887:PHE:CE1	2.41	0.54
1:B:1046:ILE:HG23	1:B:1146:TYR:HE2	1.71	0.54
2:C:1:DT:H2'	2:C:2:DA:C8	2.42	0.54
1:A:1116:ILE:HD12	1:A:1116:ILE:H	1.73	0.54
1:A:329:SER:HB3	1:A:464:PHE:HA	1.90	0.54
1:A:553:TYR:CE1	1:A:835:MET:SD	3.01	0.54
1:A:653:ARG:HG3	1:A:923:TYR:CE2	2.42	0.54
1:B:876:THR:HB	2:C:11:DOC:H2"	1.90	0.54
1:A:244:GLU:HG2	1:A:531:LEU:HB2	1.90	0.54
1:A:581:ILE:HG23	1:A:621:LEU:HD22	1.90	0.53
1:A:628:ASN:ND2	1:A:628:ASN:H	2.05	0.53
1:B:982:LYS:HB3	2:C:10:DT:H5"	1.91	0.53
1:A:314:MET:HG2	1:A:347:PHE:CZ	2.44	0.53
1:A:285:VAL:HG13	1:A:371:PRO:HA	1.90	0.53
1:B:454:LEU:CD1	1:B:459:MET:HG2	2.39	0.53
1:A:295:LYS:N	1:A:460:THR:OG1	2.33	0.53
1:B:994:LEU:HD12	1:B:1045:LEU:CD2	2.39	0.53
1:A:347:PHE:CD2	1:A:475:VAL:HG23	2.44	0.53
1:A:865:VAL:O	1:A:869:GLY:N	2.42	0.53
1:A:1039:ASP:O	1:A:1043:VAL:HG23	2.10	0.53
1:B:1093:ILE:CD1	1:B:1145:TYR:CD1	2.91	0.52
1:A:617:ILE:HG12	1:A:891:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:565:VAL:HG21	1:A:1006:PHE:CD1	2.44	0.52
1:B:210:LEU:HD21	1:B:241:ASP:HA	1.91	0.52
1:A:291:ILE:O	1:A:291:ILE:HG13	2.08	0.52
1:A:875:ASP:O	1:A:877:ASP:N	2.42	0.52
1:B:645:TYR:HB2	1:B:646:PRO:HD3	1.92	0.52
1:A:1029:VAL:HA	1:A:1036:MET:HE3	1.92	0.52
1:B:298:LEU:O	1:B:1077:LEU:CD2	2.58	0.52
1:B:485:TYR:HA	1:B:489:VAL:HG12	1.91	0.52
1:B:1100:ALA:HB1	1:B:1101:PRO:HD2	1.91	0.52
1:B:651:THR:CG2	1:B:941:THR:H	2.22	0.52
1:B:460:THR:HB	1:B:461:PRO:HD3	1.92	0.52
1:B:875:ASP:O	1:B:877:ASP:N	2.42	0.52
1:B:261:VAL:HB	1:B:497:CYS:HB3	1.92	0.52
1:B:732:VAL:HA	1:B:735:ILE:HD12	1.91	0.52
1:A:990:GLY:HA3	1:A:1049:ASN:O	2.09	0.51
1:B:248:PRO:HB2	1:B:251:VAL:HG12	1.92	0.51
1:B:653:ARG:HG3	1:B:923:TYR:CE2	2.45	0.51
1:A:76:VAL:HA	1:A:266:LYS:HA	1.92	0.51
1:B:485:TYR:CE2	1:B:490:HIS:HB2	2.45	0.51
1:A:1094:SER:HB3	1:A:1107:ILE:HD12	1.92	0.51
1:B:1119:LYS:O	1:B:1123:LEU:HD12	2.10	0.51
1:B:591:ALA:HA	1:B:912:TYR:HD2	1.76	0.51
1:A:567:ARG:NH2	1:A:570:LEU:HD11	2.25	0.51
1:B:990:GLY:HA3	1:B:1049:ASN:O	2.11	0.51
1:B:992:LEU:HD22	1:B:1149:ARG:CZ	2.41	0.51
1:B:982:LYS:HD2	2:C:11:DOC:OP2	2.10	0.51
1:A:596:VAL:HG21	1:A:604:VAL:HG22	1.93	0.51
1:B:1145:TYR:OH	1:B:1149:ARG:NH1	2.44	0.51
1:B:691:PRO:CG	1:B:742:TYR:CE1	2.92	0.51
3:D:11:DC:H2"	3:D:12:DG:C8	2.45	0.51
1:A:556:GLY:HA3	1:A:876:THR:HG22	1.93	0.51
1:A:968:ARG:HA	1:A:982:LYS:O	2.11	0.51
1:B:365:HIS:O	1:B:369:VAL:HG22	2.11	0.51
1:A:696:GLU:HA	1:A:699:MET:HE3	1.94	0.50
1:B:723:PHE:CZ	1:B:731:GLN:HG3	2.46	0.50
1:A:46:ILE:HD13	1:A:403:GLY:HA2	1.92	0.50
1:A:52:PHE:CE1	1:A:128:SER:HB2	2.47	0.50
1:A:607:VAL:HA	1:A:895:LEU:HA	1.92	0.50
1:A:864:LEU:HD12	1:A:913:ARG:HD2	1.93	0.50
1:B:242:ILE:O	1:B:242:ILE:HG13	2.11	0.50
1:A:887:PHE:CD2	1:A:888:PRO:HD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ILE:HG12	1:A:891:TYR:CZ	2.46	0.50
1:B:644:MET:SD	1:B:877:ASP:HB3	2.52	0.50
1:B:306:ASP:O	1:B:390:ARG:NH2	2.45	0.50
1:B:608:THR:OG1	1:B:609:ASN:N	2.45	0.50
1:B:548:LEU:HD23	1:B:689:PHE:HB3	1.94	0.50
1:A:961:GLU:HB2	1:A:1179:TRP:CD2	2.47	0.50
1:B:443:THR:HG23	1:B:447:LEU:HD12	1.93	0.50
1:A:1164:LEU:O	1:A:1164:LEU:HG	2.11	0.50
1:B:121:PHE:HB2	1:B:129:PHE:CE2	2.47	0.49
1:B:291:ILE:HG13	1:B:291:ILE:O	2.11	0.49
1:B:356:VAL:HG22	1:B:394:HIS:CD2	2.47	0.49
1:B:893:PHE:HB2	1:B:901:LEU:HB2	1.94	0.49
1:A:548:LEU:HD23	1:A:689:PHE:HB3	1.93	0.49
1:B:904:SER:OG	1:B:907:CYS:HB2	2.12	0.49
1:A:88:SER:O	1:A:90:GLU:N	2.46	0.49
1:A:558:VAL:HG23	1:A:874:LEU:O	2.12	0.49
1:A:636:ILE:HG12	1:A:882:ILE:HD11	1.95	0.49
2:C:5:DC:H2"	2:C:6:DG:C8	2.47	0.49
1:B:1116:ILE:HB	1:B:1117:PRO:CD	2.38	0.49
1:B:246:ASP:OD1	1:B:840:ARG:NH2	2.44	0.49
1:A:628:ASN:ND2	1:A:628:ASN:N	2.60	0.49
1:A:978:LEU:HD21	1:A:981:LEU:HD22	1.95	0.49
1:B:121:PHE:HB2	1:B:129:PHE:CD2	2.48	0.49
1:B:1151:GLY:O	1:B:1155:GLN:HG3	2.13	0.49
1:B:354:ASP:OD1	1:B:355:GLU:N	2.45	0.49
1:A:426:VAL:HA	1:A:430:SER:HB3	1.93	0.48
1:B:485:TYR:HA	1:B:489:VAL:CG1	2.43	0.48
1:A:380:ASP:HB2	1:A:421:ASP:OD2	2.14	0.48
1:A:868:VAL:CG2	1:A:887:PHE:CE1	2.91	0.48
1:B:644:MET:O	1:B:648:ILE:N	2.47	0.48
1:B:644:MET:HE3	1:B:854:GLY:HA2	1.95	0.48
1:A:569:ASP:C	1:A:570:LEU:HD12	2.33	0.48
1:A:1151:GLY:O	1:A:1155:GLN:HG2	2.13	0.48
1:B:160:LEU:HD11	1:B:206:LEU:HD21	1.96	0.47
1:B:897:ASN:N	1:B:897:ASN:OD1	2.47	0.47
1:B:1112:PHE:CD1	1:B:1137:ILE:CD1	2.98	0.47
1:B:1181:LYS:O	1:B:1184:ILE:HG13	2.15	0.47
1:B:910:LEU:O	1:B:914:VAL:HG23	2.13	0.47
1:A:296:PRO:HD3	1:A:306:ASP:OD1	2.13	0.47
1:A:510:LYS:HD3	1:A:514:THR:HG21	1.95	0.47
1:A:875:ASP:OD1	1:A:876:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:VAL:HG21	1:A:887:PHE:HE1	1.78	0.47
1:B:924:GLN:HG2	1:B:936:THR:HG22	1.95	0.47
1:A:649:MET:HA	1:A:654:LEU:HB2	1.96	0.47
1:B:293:THR:HG22	1:B:308:ILE:HA	1.96	0.47
1:A:787:LEU:HD23	1:A:787:LEU:HA	1.69	0.47
1:B:552:THR:O	1:B:686:ARG:N	2.44	0.47
1:B:1119:LYS:HB2	1:B:1119:LYS:HZ3	1.78	0.47
1:B:1145:TYR:CZ	1:B:1149:ARG:HD2	2.50	0.47
1:B:303:SER:O	1:B:390:ARG:NH2	2.47	0.47
1:B:654:LEU:HD23	1:B:762:VAL:HG11	1.96	0.47
1:B:1129:ASP:OD1	1:B:1131:SER:OG	2.28	0.47
1:A:953:MET:SD	1:A:955:LEU:HD11	2.55	0.47
1:B:293:THR:HG21	1:B:386:PHE:CE2	2.50	0.47
1:A:836:ARG:HB2	3:T:5:DT:H4'	1.97	0.46
1:A:141:ILE:HG13	1:A:191:LEU:HD11	1.96	0.46
1:B:50:MET:HE1	1:B:370:ARG:HA	1.96	0.46
3:T:6:DG:H2'	3:T:7:DA:C8	2.51	0.46
2:C:10:DT:H2''	2:C:11:DOC:H5'	1.97	0.46
1:B:577:ASP:OD1	1:B:579:SER:HB3	2.16	0.46
1:B:641:VAL:HA	1:B:943:PHE:O	2.15	0.46
1:A:968:ARG:HG3	1:A:983:GLY:HA3	1.96	0.46
1:B:551:GLU:HG3	1:B:844:MET:HE1	1.98	0.46
1:B:876:THR:CB	2:C:11:DOC:H2''	2.46	0.46
1:A:1016:TYR:HA	1:A:1019:VAL:HG12	1.98	0.46
1:B:1023:CYS:HB3	1:B:1154:ILE:CD1	2.45	0.46
1:B:213:ASN:HD21	1:B:237:HIS:HA	1.81	0.46
1:B:660:LYS:O	1:B:761:ILE:HD11	2.16	0.46
1:A:676:THR:OG1	1:A:677:CYS:N	2.48	0.46
1:A:747:TYR:C	1:A:749:ARG:H	2.19	0.46
1:B:298:LEU:O	1:B:1077:LEU:HD23	2.16	0.46
1:B:86:LEU:HD23	1:B:115:SER:HA	1.98	0.46
1:A:653:ARG:HG3	1:A:923:TYR:CZ	2.51	0.46
1:B:38:LEU:HD23	1:B:39:ASN:H	1.81	0.45
1:B:887:PHE:CD1	1:B:888:PRO:HD2	2.52	0.45
1:B:558:VAL:HG23	1:B:874:LEU:O	2.16	0.45
1:B:887:PHE:CG	1:B:888:PRO:HD2	2.51	0.45
1:B:924:GLN:CG	1:B:936:THR:HG22	2.46	0.45
1:B:1111:ILE:HD12	1:B:1126:TRP:CZ3	2.51	0.45
1:B:501:PRO:HD2	1:B:518:MET:HB3	1.98	0.45
1:B:580:ALA:HA	1:B:867:ARG:NH2	2.28	0.45
1:A:332:ILE:CG2	1:A:351:ASN:HD21	2.23	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MET:CE	1:A:50:MET:HA	2.45	0.45
1:A:680:LYS:O	1:A:681:LEU:HD23	2.16	0.45
1:A:874:LEU:HD12	1:A:879:ILE:HG12	1.98	0.45
1:B:458:LEU:O	1:B:462:TYR:CD1	2.70	0.45
1:B:586:GLN:O	1:B:589:PRO:HD2	2.16	0.45
1:A:1100:ALA:O	1:A:1105:ARG:NH1	2.45	0.45
1:A:287:MET:HB3	1:A:287:MET:HE2	1.74	0.45
1:A:485:TYR:CE2	1:A:490:HIS:HB2	2.51	0.45
1:A:585:LEU:HD23	1:A:588:LEU:HD21	1.99	0.45
1:B:287:MET:HA	1:B:314:MET:O	2.17	0.45
1:A:1073:LEU:HD13	1:A:1108:PRO:HB3	1.99	0.44
1:A:456:PRO:HA	1:A:459:MET:HE2	1.99	0.44
1:A:1147:ARG:NH2	1:A:1173:ARG:O	2.50	0.44
1:A:689:PHE:CE2	1:A:752:VAL:HB	2.52	0.44
1:B:1059:TYR:O	1:B:1062:GLN:HB2	2.17	0.44
1:B:1121:SER:O	1:B:1124:ARG:HB2	2.17	0.44
1:B:1056:LEU:HD21	1:B:1071:ARG:HG3	2.00	0.44
1:B:1029:VAL:HA	1:B:1036:MET:HG3	1.99	0.44
1:B:1029:VAL:HG13	1:B:1037:LEU:HD21	2.00	0.44
1:B:907:CYS:SG	1:B:946:VAL:HG13	2.57	0.44
1:A:876:THR:OG1	2:P:11:DOC:H2"	2.17	0.44
1:A:1083:LYS:HG2	1:A:1084:ASP:OD1	2.17	0.44
1:A:177:MET:HE2	1:A:177:MET:HB3	1.68	0.44
1:A:261:VAL:HB	1:A:497:CYS:HB3	1.99	0.44
1:A:78:TRP:CZ3	1:A:80:THR:HG22	2.53	0.44
1:A:895:LEU:HD23	1:A:895:LEU:H	1.82	0.44
1:B:1119:LYS:HZ2	1:B:1119:LYS:HB2	1.75	0.44
1:B:1176:HIS:CG	1:B:1180:LEU:HD23	2.52	0.44
1:B:560:SER:HB2	1:B:966:LYS:HG2	2.00	0.44
1:B:737:LYS:O	1:B:739:LEU:N	2.44	0.44
1:A:44:ASP:OD1	1:A:54:ARG:NH1	2.48	0.44
1:A:994:LEU:HD21	1:A:1150:LEU:HD12	1.99	0.44
1:A:195:ASN:OD1	1:A:197:ASN:N	2.50	0.44
1:A:571:LYS:N	1:A:633:LEU:HD23	2.33	0.44
1:B:152:VAL:HG13	1:B:189:ILE:HD11	2.00	0.44
1:A:539:ILE:HD12	1:A:728:TYR:CD2	2.53	0.44
1:B:298:LEU:O	1:B:1077:LEU:HD21	2.18	0.44
1:B:294:THR:HA	1:B:309:MET:HE2	2.00	0.44
1:B:652:ASN:HB2	1:B:654:LEU:HG	2.00	0.44
1:A:1011:THR:O	1:A:1015:CYS:N	2.49	0.43
1:A:560:SER:HB2	1:A:966:LYS:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:HD12	1:A:120:TYR:O	2.19	0.43
1:B:581:ILE:HD11	1:B:621:LEU:O	2.19	0.43
1:A:1184:ILE:HD12	1:A:1185:ALA:N	2.34	0.43
1:B:78:TRP:CZ3	1:B:80:THR:HG22	2.53	0.43
1:B:496:LEU:HB3	1:B:507:THR:HG21	1.99	0.43
1:B:78:TRP:CE3	1:B:80:THR:HG22	2.54	0.43
1:B:835:MET:HE2	1:B:835:MET:HB3	1.83	0.43
1:B:959:LYS:O	1:B:1179:TRP:NE1	2.49	0.43
1:A:443:THR:HG23	1:A:447:LEU:HD12	1.99	0.43
1:A:592:LEU:O	1:A:596:VAL:HG13	2.18	0.43
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.53	0.43
1:B:677:CYS:O	1:B:677:CYS:SG	2.76	0.43
1:B:761:ILE:O	1:B:761:ILE:HD12	2.18	0.43
1:A:1094:SER:OG	1:A:1105:ARG:HB3	2.18	0.43
1:B:968:ARG:HA	1:B:982:LYS:O	2.19	0.43
1:B:950:TYR:HB3	1:B:972:PHE:O	2.19	0.43
1:B:1116:ILE:CB	1:B:1117:PRO:HD3	2.46	0.43
1:B:865:VAL:HA	1:B:868:VAL:CG1	2.48	0.43
1:B:591:ALA:HA	1:B:912:TYR:CD2	2.53	0.43
1:B:68:ASP:O	1:B:72:ILE:HD12	2.19	0.43
3:D:6:DG:H2''	3:D:7:DA:H5'	2.00	0.43
1:A:295:LYS:HB3	1:A:295:LYS:HE3	1.95	0.42
1:A:287:MET:HE1	1:A:366:ILE:HG12	2.01	0.42
1:A:438:GLY:O	1:A:442:VAL:HG23	2.18	0.42
1:A:789:LYS:HE3	1:A:789:LYS:HB3	1.82	0.42
1:B:314:MET:HE2	1:B:314:MET:HB2	1.92	0.42
1:B:485:TYR:CD1	1:B:489:VAL:HG13	2.55	0.42
1:B:552:THR:HG23	3:D:7:DA:OP1	2.19	0.42
1:B:606:LYS:O	1:B:895:LEU:HD12	2.19	0.42
1:B:940:ASN:HD21	1:B:942:ILE:HD12	1.84	0.42
1:A:1092:ILE:HG12	1:A:1109:VAL:HG12	2.01	0.42
1:A:404:PHE:CE2	1:A:414:SER:HB3	2.54	0.42
1:A:493:ILE:HA	1:A:493:ILE:HD13	1.80	0.42
1:A:992:LEU:HD23	1:A:995:ILE:HD12	2.01	0.42
1:B:1097:PRO:O	1:B:1100:ALA:HB3	2.20	0.42
1:B:121:PHE:HB3	1:B:129:PHE:CE2	2.54	0.42
1:A:1050:ARG:HH11	1:A:1050:ARG:HB3	1.85	0.42
1:A:633:LEU:HA	1:A:633:LEU:HD23	1.82	0.42
1:A:655:GLN:HG3	1:A:771:VAL:CG2	2.49	0.42
1:A:655:GLN:HG3	1:A:771:VAL:HG23	2.02	0.42
1:B:607:VAL:CG2	1:B:894:THR:O	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:845:GLU:O	1:B:849:ILE:HD12	2.19	0.42
1:B:644:MET:HE1	1:B:854:GLY:HA2	1.81	0.42
1:A:680:LYS:HE3	1:A:680:LYS:HB3	1.93	0.42
1:B:1138:ARG:HH21	1:B:1138:ARG:CG	2.14	0.42
1:B:121:PHE:CD2	1:B:129:PHE:CZ	3.08	0.42
1:A:645:TYR:CD2	4:A:1301:DTP:H2'1	2.55	0.42
1:A:547:LEU:HD23	1:A:548:LEU:N	2.35	0.42
1:A:615:ASN:HA	1:A:618:THR:HG22	2.00	0.42
1:A:1133:GLU:O	1:A:1135:LEU:HD22	2.20	0.42
1:B:645:TYR:O	1:B:646:PRO:C	2.56	0.41
1:A:332:ILE:CG2	1:A:349:ILE:HG21	2.50	0.41
1:A:334:ASP:HA	1:A:349:ILE:CD1	2.50	0.41
1:A:709:PHE:HE2	1:A:723:PHE:HB2	1.84	0.41
1:A:1092:ILE:HD13	1:A:1092:ILE:HA	1.79	0.41
1:A:1137:ILE:HD12	1:A:1137:ILE:H	1.86	0.41
1:A:585:LEU:HA	1:A:588:LEU:HD21	2.02	0.41
1:A:862:ARG:HA	1:A:865:VAL:HG22	2.02	0.41
1:B:1002:ILE:HG12	1:B:1158:ILE:HD11	2.02	0.41
1:B:243:ARG:HB3	1:B:243:ARG:HE	1.76	0.41
1:A:686:ARG:HD3	1:A:755:ILE:HG22	2.02	0.41
1:B:407:ASP:OD2	1:B:413:LYS:NZ	2.53	0.41
1:B:496:LEU:HA	1:B:496:LEU:HD12	1.82	0.41
1:B:1178:ASP:HB3	1:B:1182:ARG:HH22	1.84	0.41
1:A:320:PHE:HD1	1:A:348:THR:OG1	2.04	0.41
1:B:1150:LEU:O	1:B:1150:LEU:HD23	2.20	0.41
2:P:5:DC:H2"	2:P:6:DG:C8	2.55	0.41
1:A:496:LEU:HB3	1:A:507:THR:HG21	2.02	0.41
1:B:958:SER:HB3	1:B:963:LYS:O	2.21	0.41
1:A:314:MET:SD	1:A:479:VAL:HA	2.61	0.41
1:A:565:VAL:HG22	1:A:954:ILE:HG13	2.02	0.41
1:A:574:PHE:CE2	1:A:882:ILE:HG23	2.48	0.41
1:B:244:GLU:OE1	1:B:252:ARG:NH2	2.54	0.41
1:B:406:PRO:HD3	1:B:412:TYR:CE2	2.56	0.41
1:B:337:TYR:CE2	1:B:476:SER:HA	2.56	0.41
1:B:489:VAL:HG23	1:B:493:ILE:HG12	2.02	0.41
1:A:581:ILE:HG23	1:A:621:LEU:CD2	2.50	0.41
1:A:1124:ARG:NE	1:A:1132:LEU:H	2.19	0.41
1:A:477:ASP:O	1:A:481:THR:HG23	2.21	0.41
1:A:554:VAL:HB	1:A:684:ALA:HB3	2.03	0.41
1:A:33:SER:O	1:A:36:GLN:N	2.52	0.41
1:A:308:ILE:N	1:A:355:GLU:OE1	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:HE2	1:A:475:VAL:HG23	1.85	0.40
1:A:51:GLY:O	1:A:128:SER:OG	2.21	0.40
1:B:781:ARG:HG3	1:B:823:HIS:HB2	2.02	0.40
1:A:552:THR:OG1	1:A:553:TYR:N	2.54	0.40
1:B:1082:VAL:HG12	1:B:1082:VAL:O	2.21	0.40
1:B:1119:LYS:CG	1:B:1123:LEU:CD1	2.99	0.40
1:A:588:LEU:HA	1:A:591:ALA:HB3	2.03	0.40
2:C:10:DT:H2"	2:C:11:DOC:H6	2.02	0.40
1:A:1087:LEU:HD23	1:A:1089:CYS:SG	2.61	0.40
1:A:319:GLY:HA3	1:A:347:PHE:CE1	2.57	0.40
1:B:1040:GLU:O	1:B:1043:VAL:HG22	2.22	0.40
1:B:568:SER:OG	1:B:951:LYS:HA	2.21	0.40
1:B:817:ASP:O	1:B:820:GLN:HG3	2.22	0.40
1:A:287:MET:CE	1:A:366:ILE:HG12	2.52	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	1097/1190 (92%)	1035 (94%)	60 (6%)	2 (0%)	47 64
1	B	1082/1190 (91%)	1012 (94%)	66 (6%)	4 (0%)	34 48
All	All	2179/2380 (92%)	2047 (94%)	126 (6%)	6 (0%)	41 56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	THR
1	B	876	THR
1	A	89	GLN
1	B	738	ARG

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Mol	Chain	Res	Type
1	B	889	GLU
1	B	710	PRO

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	867/1066 (81%)	841 (97%)	26 (3%)	41	59
1	B	836/1066 (78%)	809 (97%)	27 (3%)	39	56
All	All	1703/2132 (80%)	1650 (97%)	53 (3%)	40	57

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	178	ASP
1	A	212	ASP
1	A	224	ASN
1	A	254	SER
1	A	301	ARG
1	A	351	ASN
1	A	368	ASP
1	A	380	ASP
1	A	390	ARG
1	A	414	SER
1	A	454	LEU
1	A	582	ASP
1	A	588	LEU
1	A	612	GLU
1	A	628	ASN
1	A	629	ILE
1	A	630	ARG
1	A	839	SER
1	A	860	MET
1	A	907	CYS

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Mol	Chain	Res	Type
1	A	1001	ASP
1	A	1044	SER
1	A	1064	SER
1	A	1076	PHE
1	A	1087	LEU
1	B	38	LEU
1	B	129	PHE
1	B	130	LYS
1	B	131	SER
1	B	243	ARG
1	B	361	ARG
1	B	383	ASP
1	B	386	PHE
1	B	414	SER
1	B	544	ASP
1	B	637	TYR
1	B	730	ASP
1	B	734	HIS
1	B	742	TYR
1	B	753	SER
1	B	831	TYR
1	B	897	ASN
1	B	904	SER
1	B	992	LEU
1	B	994	LEU
1	B	1033	HIS
1	B	1050	ARG
1	B	1064	SER
1	B	1095	SER
1	B	1118	ILE
1	B	1119	LYS
1	B	1178	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	ASN
1	A	360	GLN
1	A	450	ASN
1	A	628	ASN
1	A	698	ASN
1	B	394	HIS

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Mol	Chain	Res	Type
1	B	915	HIS
1	B	940	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DOC	P	11	3,2	14,19,20	4.41	10 (71%)	13,26,29	1.92	3 (23%)
2	DOC	C	11	3,2	14,19,20	4.46	10 (71%)	13,26,29	1.98	3 (23%)

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
2	DOC	P	11	3,2	-	2/4/18/19	0/2/2/2
2	DOC	C	11	3,2	-	3/4/18/19	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	DOC	O4'-C4'	8.36	1.61	1.44
2	P	11	DOC	O4'-C4'	8.18	1.60	1.44
2	C	11	DOC	C6-N1	7.20	1.44	1.35
2	P	11	DOC	C6-N1	6.96	1.44	1.35
2	P	11	DOC	O4'-C1'	-6.88	1.26	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	DOC	O4'-C1'	-6.52	1.27	1.42
2	C	11	DOC	C2-N3	5.56	1.49	1.38
2	P	11	DOC	C2-N3	5.31	1.48	1.38
2	C	11	DOC	C4-N3	5.20	1.43	1.35
2	P	11	DOC	C4-N3	4.97	1.43	1.35
2	C	11	DOC	C6-C5	4.47	1.47	1.38
2	P	11	DOC	C6-C5	4.39	1.47	1.38
2	P	11	DOC	C3'-C4'	-3.83	1.32	1.52
2	C	11	DOC	C3'-C4'	-3.55	1.33	1.52
2	C	11	DOC	C5-C4	2.78	1.47	1.41
2	P	11	DOC	C5-C4	2.76	1.47	1.41
2	C	11	DOC	C2'-C1'	2.48	1.57	1.51
2	C	11	DOC	C4-N4	2.47	1.42	1.35
2	P	11	DOC	C4-N4	2.33	1.42	1.35
2	P	11	DOC	C2'-C1'	2.33	1.57	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	11	DOC	C2-N3-C4	4.44	120.85	116.34
2	C	11	DOC	C2-N3-C4	4.43	120.83	116.34
2	P	11	DOC	C3'-C2'-C1'	3.36	106.66	102.78
2	P	11	DOC	C4'-O4'-C1'	-3.03	106.95	109.81
2	C	11	DOC	C3'-C2'-C1'	2.82	106.03	102.78
2	C	11	DOC	N4-C4-N3	2.81	120.93	116.49

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	11	DOC	C3'-C4'-C5'-O5'
2	P	11	DOC	O4'-C4'-C5'-O5'
2	C	11	DOC	C3'-C4'-C5'-O5'
2	C	11	DOC	O4'-C4'-C5'-O5'
2	C	11	DOC	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	P	11	DOC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	11	DOC	5	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DTP	A	1301	5	26,32,32	2.78	7 (26%)	30,50,50	2.34	5 (16%)
4	DTP	B	1301	5	26,32,32	2.72	7 (26%)	30,50,50	2.49	4 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DTP	A	1301	5	-	3/18/34/34	0/3/3/3
4	DTP	B	1301	5	-	4/18/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	DTP	O4'-C4'	8.22	1.63	1.45
4	B	1301	DTP	O4'-C4'	8.14	1.63	1.45
4	A	1301	DTP	C3'-C4'	-7.86	1.31	1.53
4	B	1301	DTP	C3'-C4'	-7.81	1.31	1.53
4	A	1301	DTP	O4'-C1'	-4.36	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	DTP	O4'-C1'	-4.19	1.32	1.42
4	A	1301	DTP	C6-N6	3.15	1.45	1.34
4	B	1301	DTP	C6-N6	3.06	1.45	1.34
4	A	1301	DTP	O3'-C3'	3.00	1.49	1.43
4	A	1301	DTP	C2-N3	2.76	1.36	1.32
4	A	1301	DTP	C5-C4	-2.65	1.33	1.40
4	B	1301	DTP	C5-C4	-2.64	1.34	1.40
4	B	1301	DTP	O3'-C3'	2.59	1.48	1.43
4	B	1301	DTP	C2-N3	2.45	1.36	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	DTP	C5-C6-N6	9.27	134.44	120.35
4	A	1301	DTP	C5-C6-N6	8.75	133.65	120.35
4	B	1301	DTP	N6-C6-N1	-6.24	105.62	118.57
4	A	1301	DTP	N6-C6-N1	-5.78	106.57	118.57
4	B	1301	DTP	N3-C2-N1	-5.65	119.85	128.68
4	A	1301	DTP	N3-C2-N1	-5.33	120.35	128.68
4	A	1301	DTP	PB-O3B-PG	-3.38	121.24	132.83
4	B	1301	DTP	PB-O3B-PG	-3.37	121.27	132.83
4	A	1301	DTP	O3G-PG-O3B	2.01	111.37	104.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

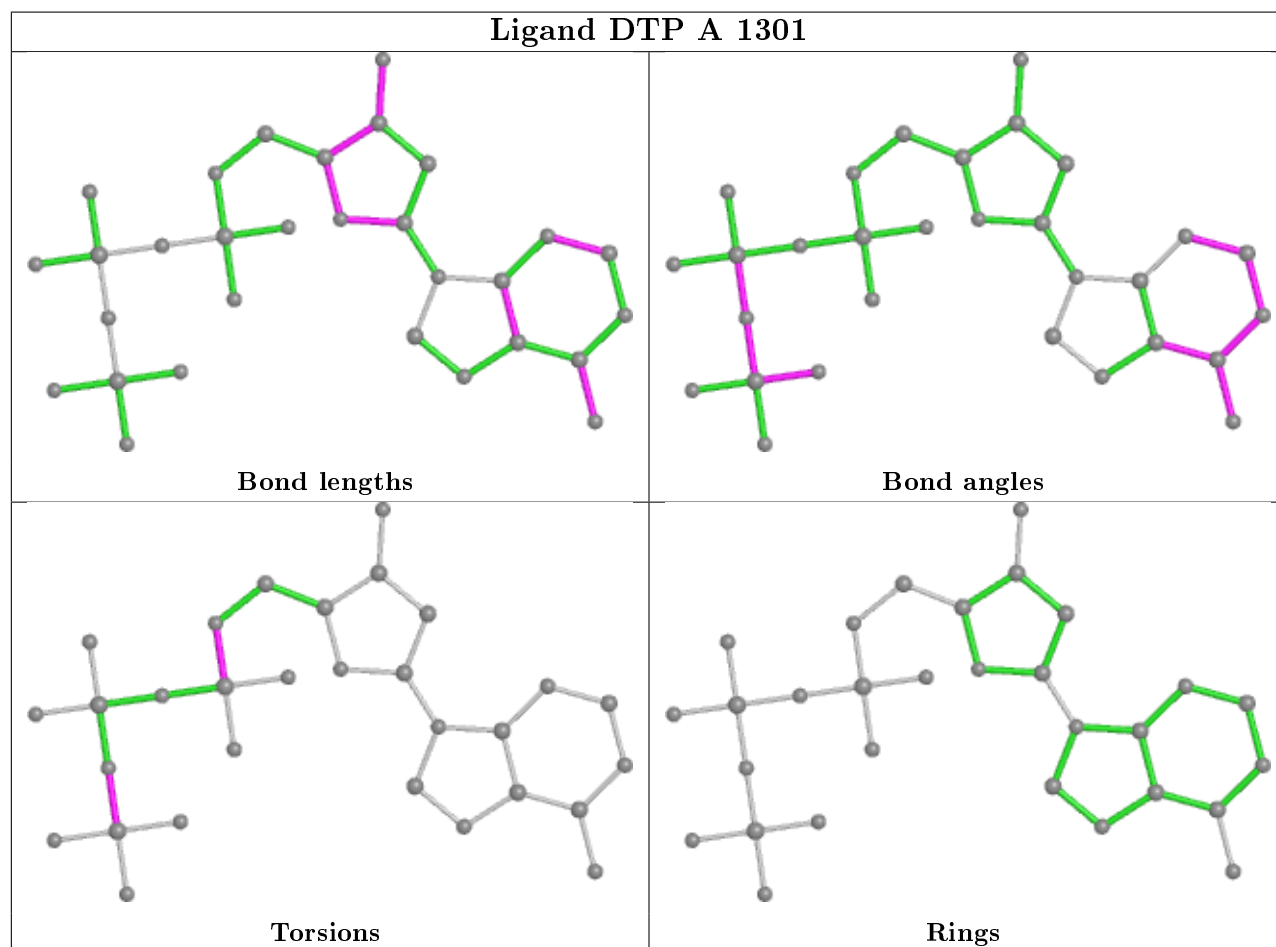
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3B-PG-O3G
4	B	1301	DTP	C5'-O5'-PA-O3A
4	B	1301	DTP	C5'-O5'-PA-O1A
4	B	1301	DTP	C5'-O5'-PA-O2A
4	A	1301	DTP	PB-O3B-PG-O2G
4	B	1301	DTP	PB-O3B-PG-O3G
4	A	1301	DTP	C5'-O5'-PA-O3A

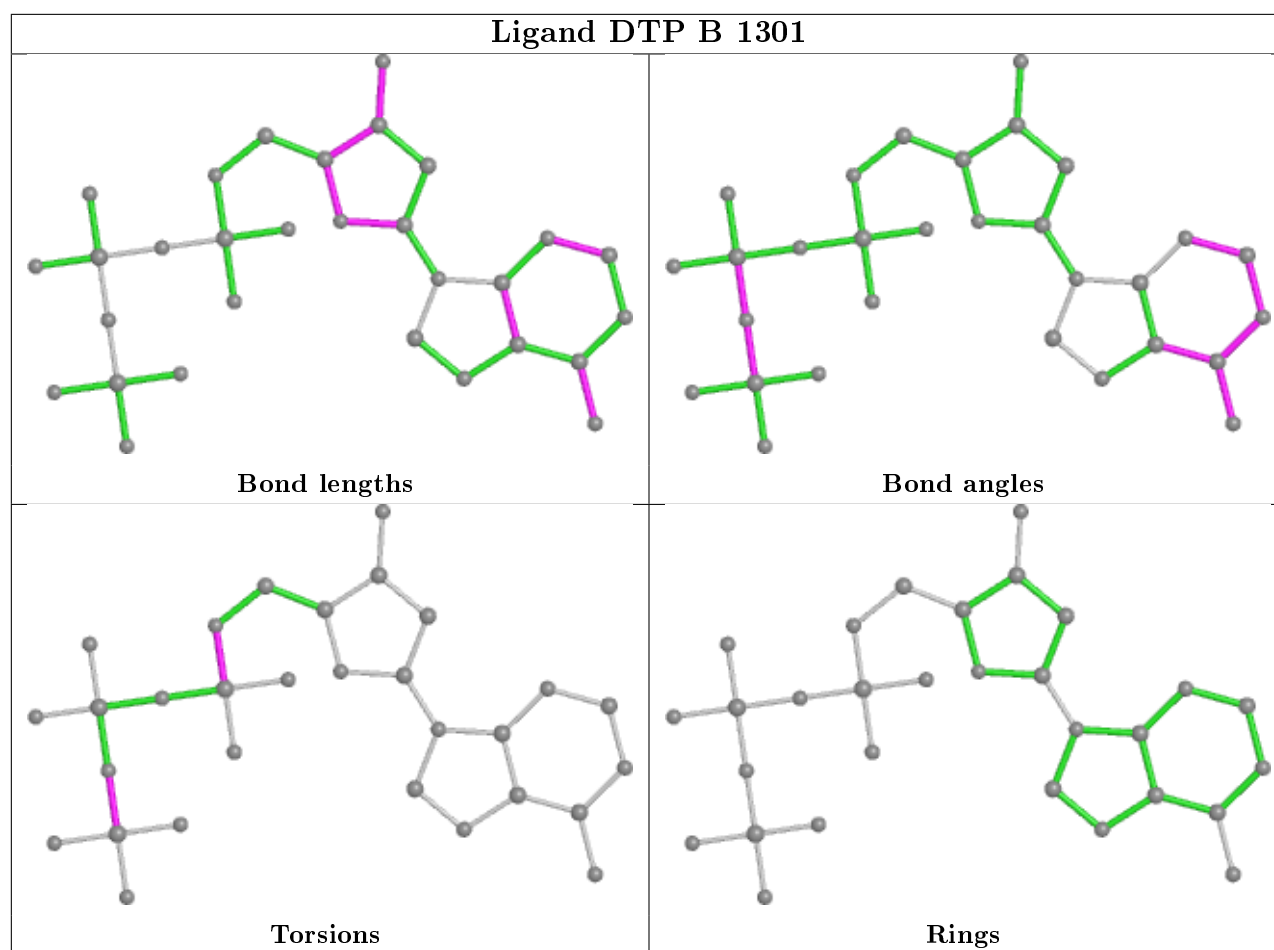
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1301	DTP	1	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	1107/1190 (93%)	0.14	28 (2%) 57 53	50, 78, 101, 119	0
1	B	1094/1190 (91%)	0.20	40 (3%) 41 38	47, 81, 105, 123	0
2	C	10/11 (90%)	-0.27	0 100 100	54, 68, 85, 87	1 (10%)
2	P	10/11 (90%)	-0.08	0 100 100	52, 65, 80, 82	1 (10%)
3	D	15/16 (93%)	-0.15	0 100 100	49, 67, 87, 99	0
3	T	15/16 (93%)	-0.11	0 100 100	48, 63, 88, 97	0
All	All	2251/2434 (92%)	0.16	68 (3%) 50 47	47, 79, 104, 123	2 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	VAL	4.9
1	A	706	ASN	4.6
1	B	64	PHE	4.5
1	B	894	THR	4.3
1	B	596	VAL	4.3
1	A	1046	ILE	4.2
1	B	235	ALA	4.1
1	B	584	LEU	4.1
1	B	548	LEU	3.7
1	B	1115	ASP	3.6
1	B	801	SER	3.6
1	B	799	ASP	3.5
1	B	539	ILE	3.5
1	B	547	LEU	3.4
1	A	723	PHE	3.4
1	B	613	ILE	3.4
1	B	1118	ILE	3.3
1	B	1070	ALA	3.3
1	B	238	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	605	ASP	3.2
1	B	734	HIS	3.1
1	B	578	PRO	3.1
1	B	592	LEU	3.1
1	A	749	ARG	3.1
1	B	1076	PHE	3.1
1	A	1030	LEU	3.1
1	B	690	PHE	3.0
1	A	610	PHE	3.0
1	A	901	LEU	3.0
1	A	747	TYR	2.9
1	A	721	LEU	2.8
1	B	1116	ILE	2.8
1	B	589	PRO	2.7
1	B	114	ILE	2.7
1	A	661	ALA	2.7
1	A	322	ILE	2.7
1	B	617	ILE	2.7
1	B	729	ALA	2.6
1	B	898	GLY	2.6
1	B	1114	ALA	2.5
1	A	637	TYR	2.5
1	B	733	ILE	2.5
1	B	1100	ALA	2.4
1	A	748	HIS	2.4
1	A	893	PHE	2.4
1	A	359	LEU	2.2
1	B	431	TYR	2.2
1	A	607	VAL	2.2
1	A	709	PHE	2.2
1	B	1044	SER	2.2
1	A	1172	PRO	2.2
1	A	480	ALA	2.2
1	B	899	LYS	2.2
1	B	308	ILE	2.2
1	B	145	ASP	2.2
1	A	743	SER	2.1
1	A	300	PHE	2.1
1	A	305	VAL	2.1
1	B	1110	ALA	2.1
1	B	430	SER	2.1
1	B	432	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	578	PRO	2.0
1	B	1046	ILE	2.0
1	A	66	ALA	2.0
1	A	347	PHE	2.0
1	B	289	PHE	2.0
1	A	160	LEU	2.0
1	B	1073	LEU	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	DOC	P	11	18/19	0.96	0.25	43,51,63,64	0
2	DOC	C	11	18/19	0.96	0.22	44,52,64,67	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

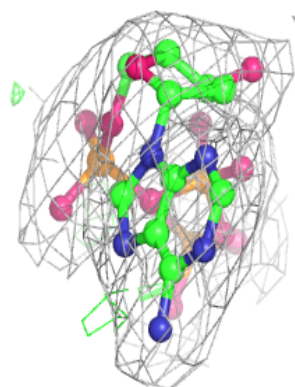
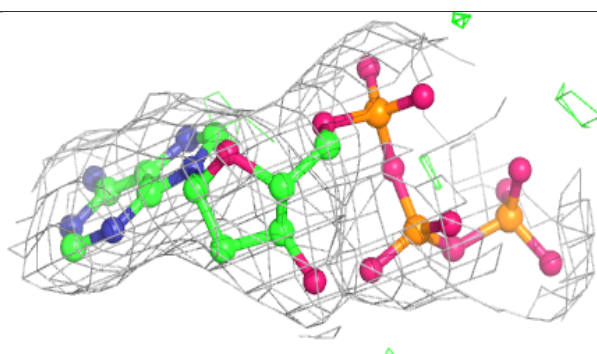
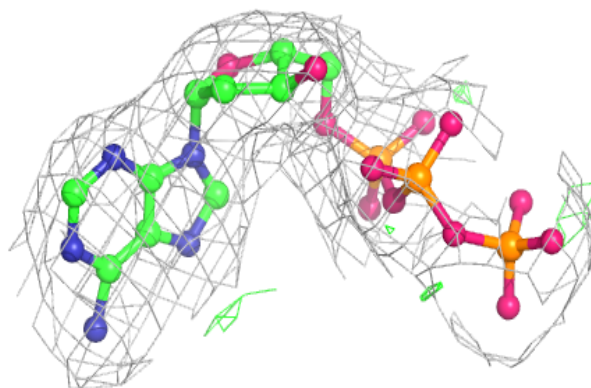
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

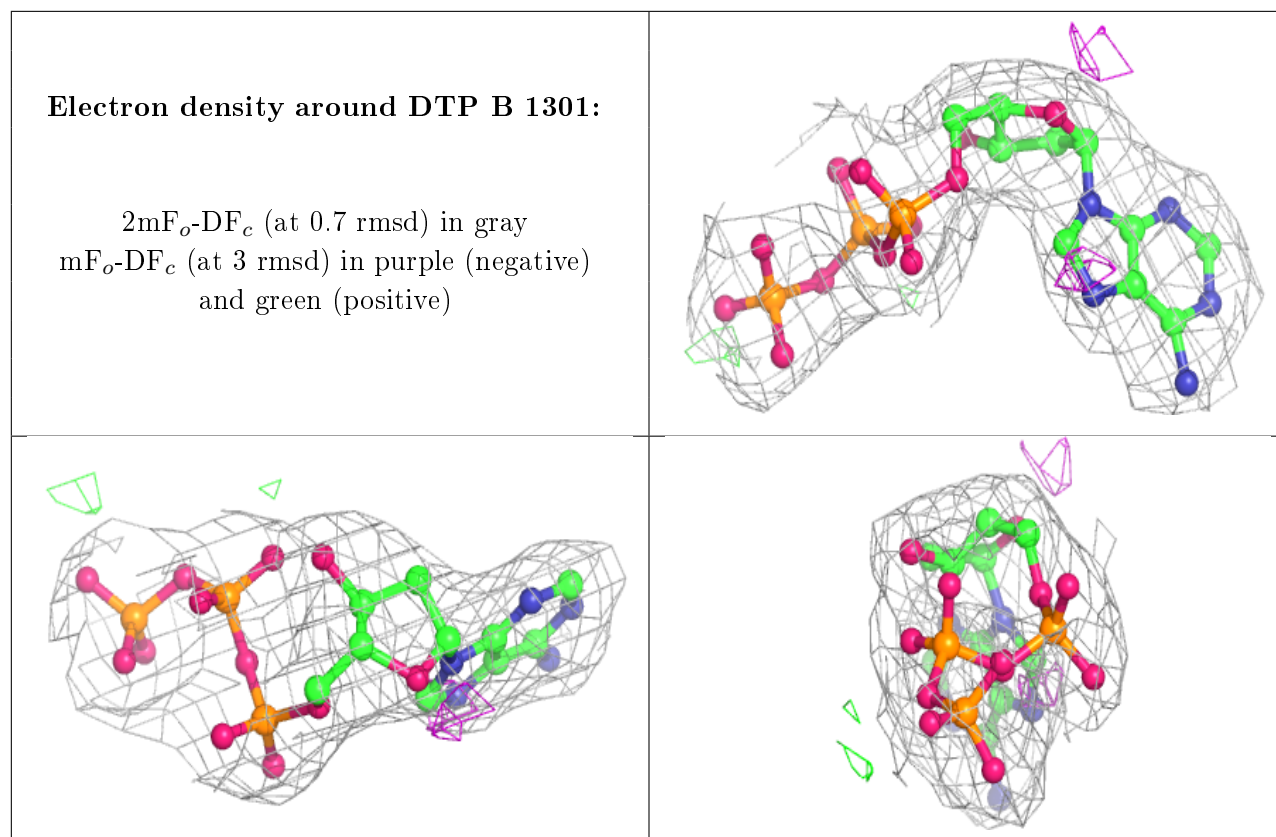
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	FE	B	1304	1/1	0.86	0.17	97,97,97,97	1
5	CA	B	1303	1/1	0.94	0.27	89,89,89,89	1
5	CA	A	1303	1/1	0.94	0.18	86,86,86,86	1
4	DTP	A	1301	30/30	0.96	0.23	44,54,62,63	0
6	FE	A	1304	1/1	0.97	0.11	109,109,109,109	1
5	CA	B	1302	1/1	0.97	0.19	55,55,55,55	0
4	DTP	B	1301	30/30	0.98	0.22	44,52,61,67	0
5	CA	A	1302	1/1	0.99	0.13	63,63,63,63	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around DTP A 1301:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.