



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:03 AM UTC

PDB ID : 6FWK / pdb_00006fwk
Title : The crystal structure of Pol2CORE-M644G in complex with DNA and an incoming nucleotide
Authors : Parkash, V.; Johansson, E.
Deposited on : 2018-03-06
Resolution : 2.50 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

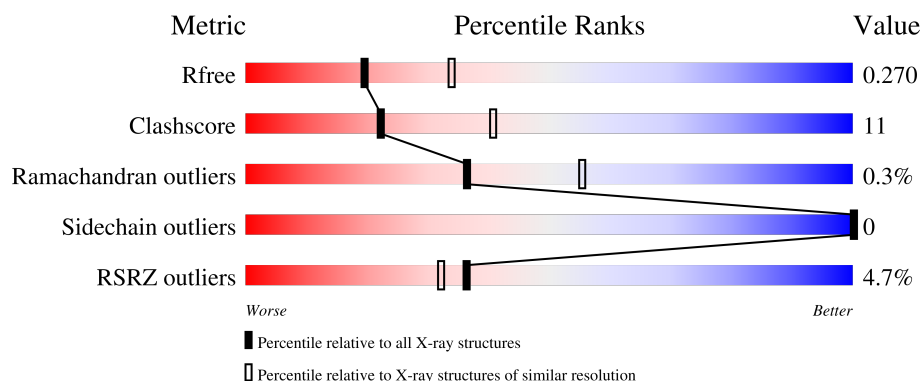
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	1191	3% 77% 16% 7%
1	B	1191	5% 72% 20% 8%
2	C	11	64% 27% 9%
2	P	11	91% 9%
3	D	15	80% 20%

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Mol	Chain	Length	Quality of chain
3	T	15	 73% 27%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18429 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	1103	Total	C	N	O	S	0	0	0
			8727	5598	1444	1643	42			
1	B	1099	Total	C	N	O	S	0	0	0
			8566	5488	1428	1610	40			

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	644	GLY	MET	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	644	GLY	MET	engineered mutation	UNP P21951

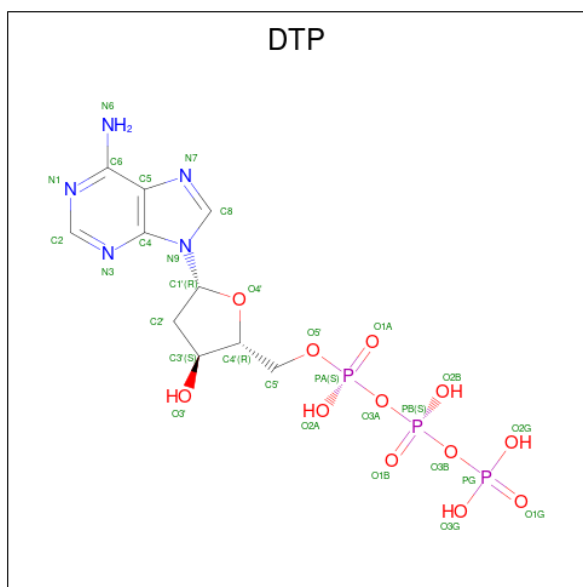
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP*(DOC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	11	Total	C	N	O	P	4	0	0
			221	106	38	66	11			
2	C	11	Total	C	N	O	P	4	0	0
			221	106	38	66	11			

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

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
			308	147	54	92	15			

- Molecule 4 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: 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 (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Ca	0	0
			2	2		
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

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

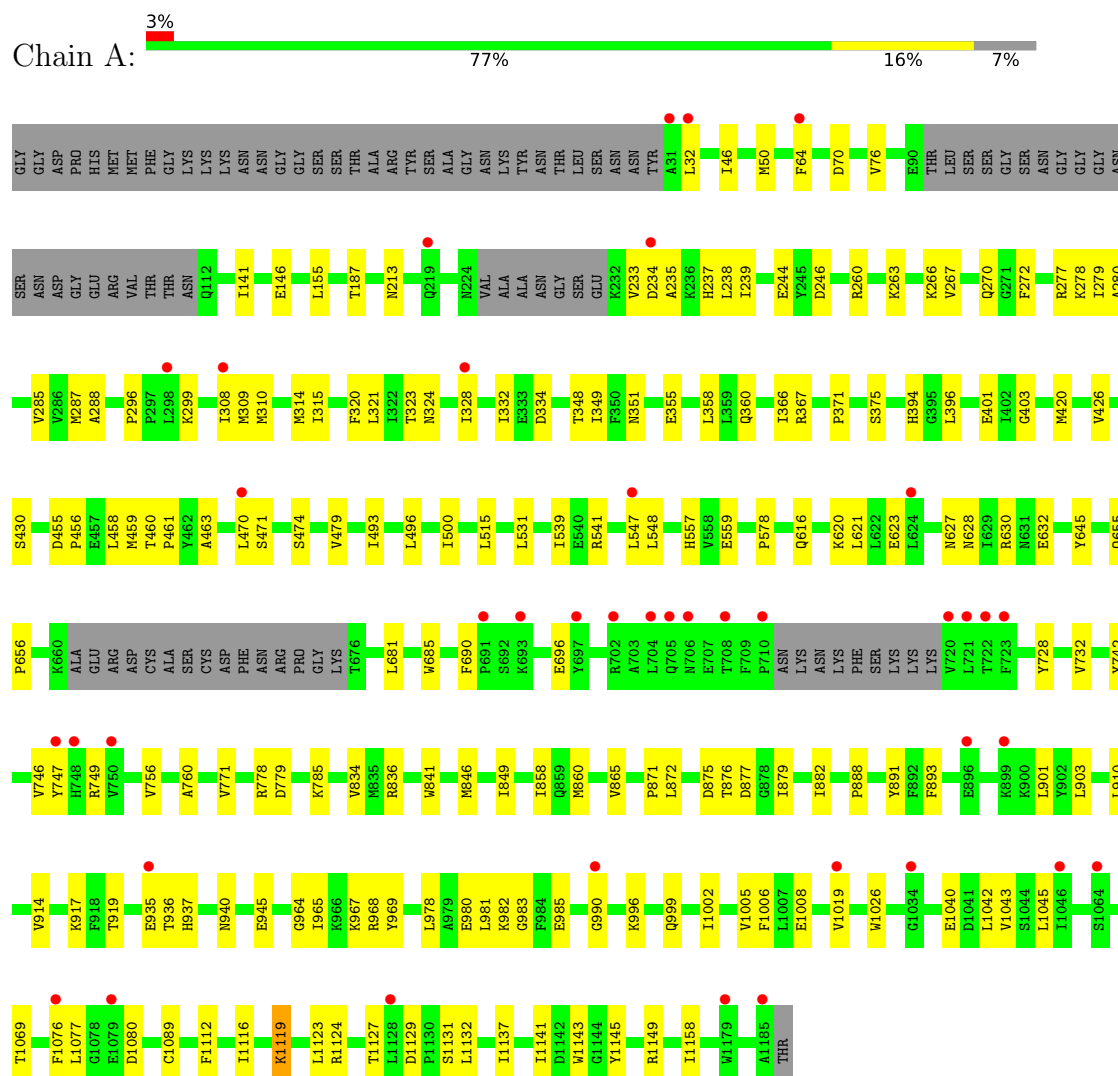
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	B	6	Total 6	O 6	0	0

3 Residue-property plots [i](#)

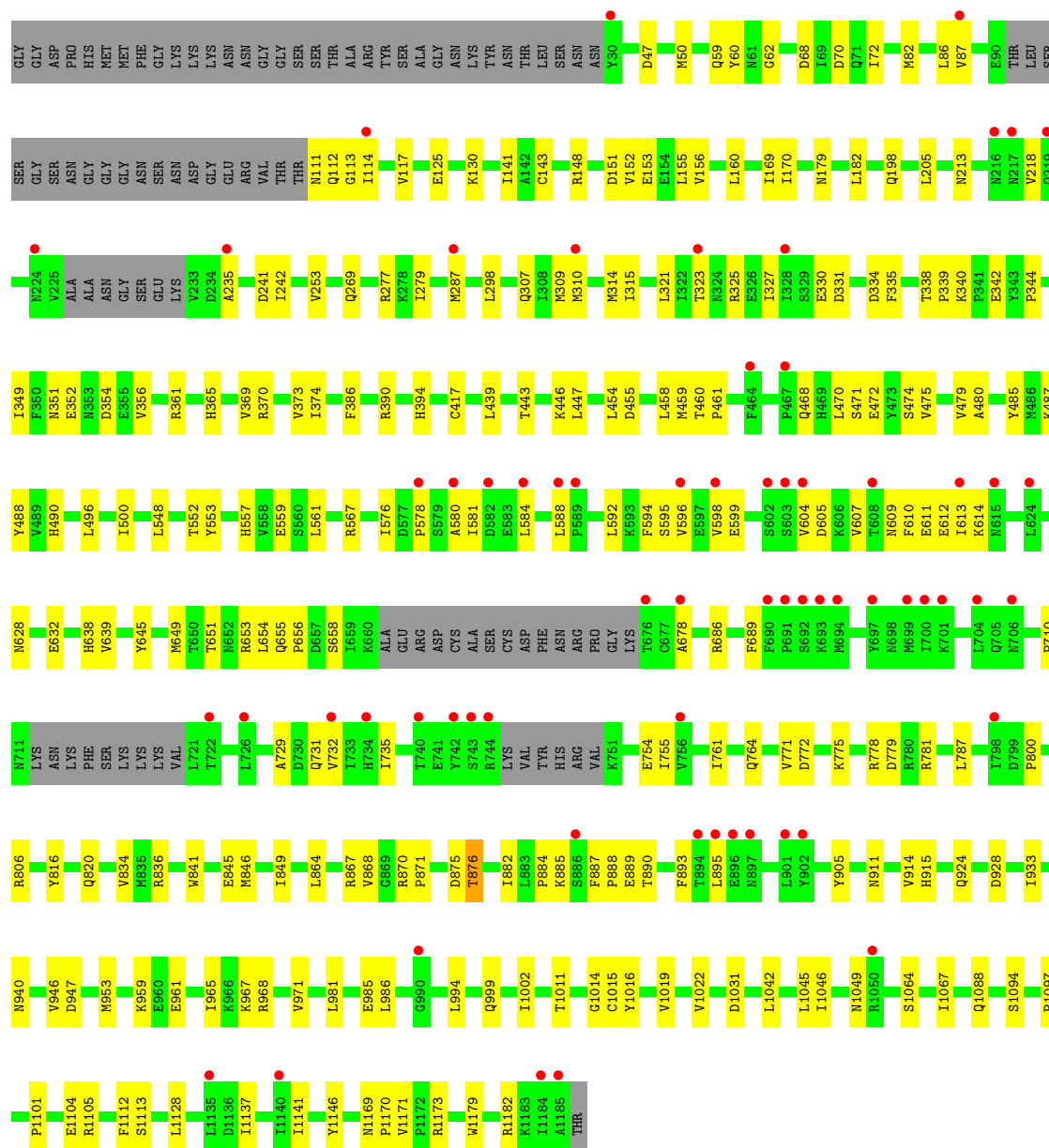
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: DNA polymerase epsilon catalytic subunit A



- Molecule 1: DNA polymerase epsilon catalytic subunit A





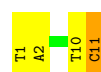
- Molecule 2: DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP*(DOC))-3')

Chain P: 91% 9%



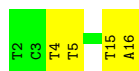
- Molecule 2: DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP*(DOC))-3')

Chain C: 64% 27% 9%



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

Chain T:  73% 27%



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

Chain D:  80% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.96Å 70.34Å 158.97Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	19.99 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.99-2.50) 99.1 (19.99-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.263 0.232 , 0.270	Depositor DCC
R_{free} test set	5420 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18429	wwPDB-VP
Average B, all atoms (Å ²)	73.0	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 54.66 % 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 3.5361e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: DTP, DOC, CA, 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	0.15	0/8929	0.35	0/12114
1	B	0.18	0/8762	0.40	0/11899
2	C	0.28	0/226	0.41	0/346
2	P	0.23	0/226	0.44	0/346
3	D	0.22	0/344	0.39	0/529
3	T	0.26	0/344	0.43	0/529
All	All	0.17	0/18831	0.38	0/25763

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	8727	0	8352	150	0
1	B	8566	0	8085	219	0
2	C	221	0	125	4	0
2	P	221	0	125	1	0
3	D	308	0	171	2	0
3	T	308	0	171	3	0
4	A	30	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	12	2	0
5	A	2	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	5	0	0	0	0
7	B	6	0	0	0	0
All	All	18429	0	17053	372	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 11.

All (372) 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:613:ILE:HD12	1:B:614:LYS:N	1.52	1.23
1:B:323:THR:OG1	1:B:351:ASN:HA	1.58	1.04
1:B:1112:PHE:CZ	1:B:1137:ILE:HD11	1.94	1.00
1:B:588:LEU:HD11	1:B:592:LEU:HG	1.43	1.00
1:B:1112:PHE:CE1	1:B:1137:ILE:HD11	2.00	0.95
1:B:613:ILE:HD12	1:B:614:LYS:H	1.33	0.93
1:B:1169:ASN:ND2	1:B:1171:VAL:H	1.66	0.92
1:B:60:TYR:H	1:B:269:GLN:HE21	1.05	0.92
1:B:1101:PRO:HD2	1:B:1104:GLU:OE1	1.72	0.90
1:B:334:ASP:HA	1:B:349:ILE:HD13	1.54	0.89
1:B:639:VAL:HG12	1:B:946:VAL:HG22	1.54	0.87
1:B:1112:PHE:CE2	1:B:1137:ILE:HD11	2.12	0.85
1:B:1011:THR:HG23	1:B:1014:GLY:H	1.42	0.84
1:B:607:VAL:HG23	1:B:895:LEU:HB3	1.58	0.84
1:B:213:ASN:OD1	1:B:213:ASN:O	1.97	0.82
1:B:86:LEU:HD23	1:B:114:ILE:O	1.78	0.82
1:A:919:THR:HG22	1:A:940:ASN:HD22	1.43	0.82
1:B:86:LEU:HD23	1:B:114:ILE:C	2.07	0.78
1:B:580:ALA:HB2	1:B:867:ARG:HE	1.48	0.78
1:A:1002:ILE:HD11	1:A:1019:VAL:HG13	1.64	0.78
1:B:578:PRO:HG3	1:B:628:ASN:ND2	1.99	0.78
1:A:308:ILE:HD12	1:A:358:LEU:CD2	2.15	0.77
1:B:800:PRO:HA	1:B:806:ARG:HD2	1.66	0.77
1:A:1119:LYS:HG2	1:A:1123:LEU:HD11	1.67	0.76
1:B:588:LEU:CD1	1:B:592:LEU:HG	2.14	0.75
1:B:60:TYR:H	1:B:269:GLN:NE2	1.83	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:TYR:N	1:B:269:GLN:HE21	1.82	0.75
1:B:86:LEU:HD22	1:B:113:GLY:C	2.11	0.74
1:B:613:ILE:HG12	1:B:893:PHE:HE1	1.53	0.74
1:A:155:LEU:HD23	1:A:155:LEU:O	1.87	0.74
1:B:323:THR:HG21	1:B:351:ASN:OD1	1.88	0.74
1:B:613:ILE:HG12	1:B:893:PHE:CE1	2.23	0.73
1:A:32:LEU:HD13	1:A:32:LEU:O	1.89	0.73
1:B:653:ARG:HD2	1:B:764:GLN:HA	1.69	0.72
1:B:1112:PHE:CD1	1:B:1137:ILE:HD11	2.24	0.72
1:B:86:LEU:CD2	1:B:114:ILE:C	2.62	0.72
1:B:588:LEU:HD12	1:B:588:LEU:O	1.90	0.72
1:B:315:ILE:HD13	1:B:369:VAL:HG11	1.71	0.71
1:B:607:VAL:HG23	1:B:895:LEU:CB	2.22	0.70
1:A:980:GLU:HB3	1:A:982:LYS:HE2	1.74	0.70
1:B:111:ASN:ND2	1:B:112:GLN:H	1.90	0.70
1:A:1019:VAL:CG1	1:A:1158:ILE:HG12	2.22	0.69
1:A:310:MET:HE1	1:A:471:SER:HA	1.73	0.69
1:A:309:MET:HE2	1:A:463:ALA:HB2	1.74	0.69
1:A:287:MET:HE1	1:A:366:ILE:HG12	1.74	0.69
1:A:285:VAL:HG13	1:A:371:PRO:HA	1.76	0.68
1:A:308:ILE:HD12	1:A:358:LEU:HD21	1.76	0.68
1:B:610:PHE:O	1:B:613:ILE:HG13	1.93	0.68
1:B:613:ILE:HD12	1:B:613:ILE:C	2.19	0.68
1:A:267:VAL:HG22	1:A:272:PHE:CE1	2.29	0.68
1:B:1112:PHE:CZ	1:B:1137:ILE:CD1	2.76	0.68
1:B:1112:PHE:CE1	1:B:1137:ILE:CD1	2.75	0.68
1:A:324:ASN:H	1:A:328:ILE:HD13	1.59	0.67
1:B:967:LYS:O	1:B:968:ARG:HG3	1.95	0.67
1:A:141:ILE:HG23	1:A:239:ILE:HG23	1.77	0.67
1:B:307:GLN:NE2	1:B:327:ILE:HD11	2.10	0.67
1:B:653:ARG:HG3	1:B:653:ARG:O	1.94	0.66
1:A:267:VAL:HG22	1:A:272:PHE:CD1	2.31	0.66
1:A:367:ARG:HD3	1:A:401:GLU:O	1.96	0.65
1:B:155:LEU:HD12	1:B:235:ALA:HB3	1.78	0.65
1:B:607:VAL:HG23	1:B:895:LEU:CA	2.26	0.64
1:A:309:MET:HE1	1:A:460:THR:HA	1.80	0.64
1:A:456:PRO:HA	1:A:459:MET:HE3	1.78	0.64
1:A:235:ALA:HA	1:A:238:LEU:HD12	1.77	0.64
1:B:1049:ASN:OD1	1:B:1088:GLN:HB3	1.97	0.64
1:B:588:LEU:HD11	1:B:592:LEU:CG	2.24	0.63
1:A:155:LEU:HD12	1:A:235:ALA:HB3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:HIS:O	1:B:369:VAL:HG13	1.99	0.63
1:A:308:ILE:CD1	1:A:358:LEU:HD22	2.29	0.62
1:B:911:ASN:HA	1:B:914:VAL:HG22	1.81	0.62
1:B:314:MET:HE1	1:B:479:VAL:HG23	1.81	0.61
1:B:1112:PHE:CD2	1:B:1137:ILE:HD11	2.35	0.61
1:A:155:LEU:HD23	1:A:155:LEU:C	2.25	0.61
1:B:655:GLN:HA	1:B:846:MET:HE2	1.82	0.61
1:B:1179:TRP:HA	1:B:1182:ARG:NH2	2.15	0.61
1:B:471:SER:O	1:B:475:VAL:HG22	2.01	0.61
1:B:953:MET:HG3	1:B:971:VAL:HG22	1.81	0.61
1:A:310:MET:HE2	1:A:474:SER:OG	2.01	0.61
1:B:1169:ASN:HD21	1:B:1171:VAL:H	1.46	0.61
1:B:548:LEU:HD23	1:B:689:PHE:HB3	1.83	0.60
1:B:1169:ASN:ND2	1:B:1171:VAL:N	2.43	0.60
1:A:308:ILE:CD1	1:A:358:LEU:CD2	2.79	0.60
1:B:632:GLU:OE2	1:B:885:LYS:N	2.35	0.60
1:B:160:LEU:HD23	1:B:205:LEU:HD12	1.84	0.60
1:B:557:HIS:NE2	1:B:559:GLU:OE1	2.30	0.59
1:B:994:LEU:HD12	1:B:1045:LEU:HD21	1.83	0.59
1:A:155:LEU:HD12	1:A:235:ALA:CB	2.32	0.59
1:A:1019:VAL:HG11	1:A:1158:ILE:HG12	1.83	0.59
1:B:1169:ASN:HD22	1:B:1169:ASN:C	2.10	0.59
1:A:893:PHE:HB2	1:A:901:LEU:HB2	1.84	0.59
1:A:324:ASN:ND2	1:A:355:GLU:HA	2.18	0.59
1:A:578:PRO:HG3	1:A:628:ASN:HD22	1.68	0.59
1:B:592:LEU:HD13	1:B:613:ILE:CD1	2.33	0.59
1:B:454:LEU:HD23	1:B:455:ASP:N	2.17	0.58
1:B:731:GLN:O	1:B:735:ILE:HG13	2.03	0.58
1:B:1031:ASP:OD2	1:B:1173:ARG:NH2	2.36	0.58
1:A:46:ILE:HD13	1:A:403:GLY:HA2	1.85	0.58
1:A:623:GLU:O	1:A:630:ARG:NH2	2.37	0.58
1:A:910:LEU:O	1:A:914:VAL:HG23	2.03	0.58
1:B:578:PRO:HA	1:B:581:ILE:HG22	1.85	0.58
1:B:613:ILE:CD1	1:B:614:LYS:N	2.47	0.58
1:A:935:GLU:OE1	1:A:936:THR:N	2.36	0.58
1:B:325:ARG:HD2	1:B:331:ASP:OD2	2.03	0.57
1:B:443:THR:HG23	1:B:447:LEU:HD12	1.86	0.57
1:A:310:MET:HE3	1:A:321:LEU:HD11	1.86	0.57
1:A:1080:ASP:OD1	1:A:1080:ASP:N	2.35	0.57
1:A:985:GLU:OE1	1:A:999:GLN:NE2	2.33	0.57
1:B:213:ASN:OD1	1:B:213:ASN:C	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:VAL:HA	1:B:895:LEU:HA	1.87	0.57
1:A:621:LEU:CD1	1:A:888:PRO:HG2	2.36	0.56
1:A:470:LEU:C	1:A:470:LEU:HD23	2.30	0.56
1:B:1042:LEU:HD11	1:B:1046:ILE:HD12	1.88	0.56
1:B:1112:PHE:CG	1:B:1137:ILE:HD11	2.40	0.56
1:B:241:ASP:OD1	1:B:242:ILE:N	2.39	0.56
1:A:557:HIS:NE2	1:A:559:GLU:OE1	2.38	0.55
1:B:152:VAL:O	1:B:156:VAL:HG13	2.06	0.55
1:B:1169:ASN:ND2	1:B:1169:ASN:C	2.64	0.55
1:B:653:ARG:NH1	1:B:924:GLN:O	2.39	0.55
1:A:1026:TRP:HZ3	1:A:1045:LEU:HD21	1.72	0.55
1:A:1137:ILE:HG22	1:A:1141:ILE:CD1	2.36	0.55
1:B:59:GLN:HA	1:B:269:GLN:NE2	2.21	0.55
1:B:592:LEU:HD13	1:B:613:ILE:HD11	1.87	0.55
1:B:999:GLN:HA	1:B:1002:ILE:HG22	1.89	0.55
1:A:328:ILE:HD12	1:A:328:ILE:H	1.72	0.55
1:B:325:ARG:NH1	1:B:330:GLU:C	2.65	0.55
1:A:308:ILE:HD12	1:A:358:LEU:HD22	1.89	0.54
1:A:968:ARG:HG3	1:A:983:GLY:HA3	1.88	0.54
1:A:1137:ILE:HG22	1:A:1141:ILE:HD11	1.89	0.54
1:A:155:LEU:C	1:A:155:LEU:CD2	2.81	0.54
1:B:141:ILE:HD13	1:B:242:ILE:HG22	1.89	0.54
1:A:627:ASN:HB2	1:A:630:ARG:NH2	2.24	0.54
1:A:872:LEU:HD11	1:A:882:ILE:HG23	1.90	0.53
1:A:426:VAL:HA	1:A:430:SER:HB3	1.89	0.53
1:A:539:ILE:HD12	1:A:728:TYR:CD2	2.43	0.53
1:B:967:LYS:HE2	2:C:10:DT:O2	2.09	0.53
1:B:179:ASN:HB3	1:B:182:LEU:HD12	1.91	0.53
1:B:1002:ILE:HD12	1:B:1022:VAL:HG13	1.90	0.53
1:A:64:PHE:HB2	1:A:270:GLN:CD	2.34	0.53
1:B:610:PHE:HD1	1:B:611:GLU:HG2	1.74	0.53
1:B:117:VAL:HG21	1:B:253:VAL:HG11	1.91	0.53
1:B:778:ARG:NH1	1:B:779:ASP:OD1	2.41	0.53
1:B:86:LEU:HD22	1:B:114:ILE:N	2.22	0.52
1:A:334:ASP:HA	1:A:349:ILE:CD1	2.39	0.52
1:A:645:TYR:CD2	4:A:1301:DTP:H2'1	2.44	0.52
1:B:68:ASP:O	1:B:72:ILE:HG13	2.09	0.52
1:A:324:ASN:HD22	1:A:355:GLU:HA	1.74	0.52
1:A:324:ASN:O	1:A:328:ILE:HD12	2.09	0.52
1:A:324:ASN:ND2	1:A:355:GLU:CA	2.73	0.52
1:B:595:SER:O	1:B:599:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:ASN:HD21	1:A:355:GLU:N	2.08	0.52
1:B:323:THR:HG1	1:B:351:ASN:HA	1.72	0.52
1:A:620:LYS:HB2	1:A:888:PRO:HG3	1.91	0.52
1:A:1145:TYR:OH	1:A:1149:ARG:NH1	2.43	0.52
1:B:356:VAL:HG22	1:B:394:HIS:CG	2.45	0.51
1:A:420:MET:HE1	1:A:493:ILE:HG21	1.93	0.51
1:B:59:GLN:OE1	1:B:269:GLN:NE2	2.44	0.51
1:B:125:GLU:HA	1:B:125:GLU:OE1	2.10	0.51
1:B:592:LEU:CD1	1:B:613:ILE:HD13	2.40	0.51
1:B:309:MET:HE1	1:B:460:THR:HA	1.91	0.51
1:A:728:TYR:O	1:A:732:VAL:HG12	2.10	0.51
1:A:858:ILE:HD11	1:A:879:ILE:HG13	1.92	0.51
1:A:865:VAL:HG12	1:A:871:PRO:HD3	1.92	0.51
1:B:639:VAL:HG12	1:B:946:VAL:CG2	2.35	0.51
1:A:547:LEU:HB3	1:A:690:PHE:HD2	1.75	0.51
1:B:87:VAL:HG12	1:B:114:ILE:O	2.10	0.51
1:B:961:GLU:HB2	1:B:1179:TRP:CD2	2.46	0.51
1:A:935:GLU:OE2	1:A:937:HIS:ND1	2.29	0.51
1:B:592:LEU:CD1	1:B:613:ILE:CD1	2.89	0.51
1:B:352:GLU:OE1	1:B:361:ARG:HD2	2.11	0.50
1:A:324:ASN:H	1:A:328:ILE:CD1	2.23	0.50
1:B:287:MET:SD	1:B:315:ILE:HG12	2.50	0.50
1:B:454:LEU:HD22	1:B:459:MET:HG3	1.93	0.50
1:B:1016:TYR:HB3	1:B:1170:PRO:HG3	1.93	0.50
1:B:576:ILE:HD11	1:B:884:PRO:HG2	1.92	0.50
1:B:592:LEU:HD22	1:B:893:PHE:HZ	1.76	0.50
1:B:60:TYR:CD2	1:B:72:ILE:HG23	2.47	0.50
1:B:875:ASP:CG	2:C:11:DOC:H4'	2.36	0.50
1:B:60:TYR:CZ	1:B:62:GLY:HA3	2.46	0.50
1:B:198:GLN:HE21	1:B:198:GLN:HA	1.77	0.50
1:A:455:ASP:OD2	1:A:455:ASP:C	2.55	0.49
1:B:349:ILE:N	1:B:349:ILE:HD12	2.26	0.49
1:B:354:ASP:OD1	1:B:354:ASP:N	2.45	0.49
1:B:459:MET:HG2	1:B:470:LEU:HD13	1.93	0.49
1:B:638:HIS:ND1	1:B:947:ASP:OD1	2.42	0.49
1:B:655:GLN:OE1	1:B:771:VAL:HG23	2.12	0.49
1:B:645:TYR:CG	4:B:1301:DTP:H2'1	2.47	0.49
1:A:742:TYR:CZ	1:A:746:VAL:HG21	2.48	0.49
1:B:307:GLN:HE21	1:B:327:ILE:HD11	1.77	0.49
1:A:146:GLU:HG2	1:A:187:THR:HB	1.94	0.49
1:A:233:VAL:HG12	1:A:234:ASP:OD2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:ASP:OD1	1:A:1131:SER:HB3	2.12	0.49
1:B:339:PRO:O	1:B:340:LYS:HG2	2.13	0.49
1:B:645:TYR:CD2	4:B:1301:DTP:H2'1	2.48	0.49
1:A:323:THR:OG1	1:A:351:ASN:HA	2.13	0.48
1:A:685:TRP:HE3	1:A:756:VAL:HG12	1.78	0.48
1:A:967:LYS:O	1:A:968:ARG:HG3	2.13	0.48
1:A:70:ASP:CG	1:A:277:ARG:HH12	2.20	0.48
1:A:1002:ILE:HD11	1:A:1019:VAL:CG1	2.40	0.48
1:B:496:LEU:HG	1:B:500:ILE:HD12	1.95	0.48
1:B:310:MET:HE2	1:B:470:LEU:HG	1.95	0.48
1:B:552:THR:OG1	1:B:553:TYR:N	2.46	0.48
1:B:656:PRO:HG2	1:B:841:TRP:HB3	1.94	0.48
1:B:454:LEU:HD23	1:B:454:LEU:C	2.38	0.48
1:A:234:ASP:OD2	1:A:237:HIS:HB2	2.13	0.48
1:A:1069:THR:HB	1:A:1089:CYS:HB3	1.96	0.48
1:B:604:VAL:HG13	1:B:605:ASP:OD1	2.14	0.48
1:A:355:GLU:OE2	1:A:394:HIS:NE2	2.36	0.47
1:B:287:MET:O	1:B:374:ILE:HA	2.14	0.47
1:B:70:ASP:CG	1:B:277:ARG:HH12	2.22	0.47
1:A:935:GLU:OE1	1:A:935:GLU:C	2.58	0.47
1:B:485:TYR:CE2	1:B:490:HIS:HB2	2.50	0.47
1:B:111:ASN:CG	1:B:112:GLN:N	2.73	0.47
1:B:834:VAL:HG21	1:B:846:MET:HE3	1.96	0.47
1:B:911:ASN:HA	1:B:914:VAL:CG2	2.43	0.47
1:A:935:GLU:OE1	1:A:936:THR:C	2.58	0.47
1:B:1169:ASN:HD22	1:B:1170:PRO:N	2.12	0.47
1:A:308:ILE:HG12	1:A:355:GLU:OE1	2.15	0.47
1:B:298:LEU:HD21	1:B:1113:SER:HB2	1.96	0.47
1:B:578:PRO:CG	1:B:628:ASN:ND2	2.75	0.47
1:B:1064:SER:HB3	1:B:1067:ILE:HD12	1.97	0.47
1:A:324:ASN:N	1:A:328:ILE:HD13	2.28	0.47
1:A:260:ARG:HB2	1:A:263:LYS:HD2	1.97	0.46
1:A:760:ALA:HB3	1:A:849:ILE:HD11	1.96	0.46
1:A:860:MET:HG3	1:A:917:LYS:HE2	1.97	0.46
1:B:875:ASP:OD2	1:B:967:LYS:HE3	2.15	0.46
1:A:969:TYR:CZ	1:A:982:LYS:HG3	2.50	0.46
1:B:651:THR:HG23	1:B:940:ASN:HA	1.97	0.46
1:A:278:LYS:HE3	1:A:278:LYS:HB3	1.78	0.46
1:B:610:PHE:O	1:B:613:ILE:CD1	2.63	0.46
1:A:287:MET:HB2	1:A:315:ILE:HG12	1.96	0.46
2:C:1:DT:H2'	2:C:2:DA:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:627:ASN:HB2	1:A:630:ARG:HH21	1.79	0.46
1:B:592:LEU:HD11	1:B:613:ILE:HD13	1.98	0.46
3:D:11:DC:H2"	3:D:12:DG:C8	2.51	0.46
1:A:539:ILE:HG22	1:A:732:VAL:HG11	1.98	0.46
1:B:578:PRO:HG3	1:B:628:ASN:HD21	1.76	0.46
1:B:1042:LEU:HD12	1:B:1042:LEU:O	2.16	0.46
1:A:656:PRO:HG2	1:A:841:TRP:HB3	1.97	0.46
1:A:1006:PHE:CE1	1:A:1019:VAL:HG21	2.51	0.46
1:B:325:ARG:CD	1:B:331:ASP:OD2	2.64	0.46
1:B:439:LEU:HD11	1:B:480:ALA:HB1	1.98	0.46
1:A:50:MET:HE1	1:A:367:ARG:HA	1.98	0.46
1:A:1123:LEU:O	1:A:1127:THR:OG1	2.29	0.46
1:A:785:LYS:NZ	1:A:945:GLU:OE1	2.47	0.45
1:B:325:ARG:HH12	1:B:330:GLU:CA	2.29	0.45
1:B:454:LEU:HD23	1:B:455:ASP:C	2.41	0.45
1:B:764:GLN:O	1:B:924:GLN:HB2	2.16	0.45
1:A:496:LEU:HG	1:A:500:ILE:HD12	1.99	0.45
1:A:320:PHE:HA	1:A:348:THR:O	2.17	0.45
1:B:334:ASP:HA	1:B:349:ILE:CD1	2.38	0.45
1:B:446:LYS:O	1:B:488:TYR:OH	2.20	0.45
1:B:653:ARG:O	1:B:653:ARG:CG	2.58	0.45
1:B:1016:TYR:HA	1:B:1019:VAL:HG22	1.99	0.45
1:B:649:MET:HA	1:B:654:LEU:HD12	1.97	0.45
1:A:541:ARG:O	1:A:548:LEU:HB2	2.16	0.45
1:A:244:GLU:HG2	1:A:531:LEU:HB2	1.98	0.45
1:B:1179:TRP:HA	1:B:1182:ARG:HH21	1.82	0.45
1:A:296:PRO:HB2	1:A:299:LYS:HB2	1.99	0.44
1:A:1040:GLU:HA	1:A:1043:VAL:HG12	1.98	0.44
1:B:458:LEU:C	1:B:461:PRO:HD2	2.42	0.44
1:B:729:ALA:O	1:B:732:VAL:HG12	2.17	0.44
1:B:59:GLN:HA	1:B:269:GLN:HE21	1.82	0.44
1:B:772:ASP:HA	1:B:775:LYS:HG2	1.98	0.44
1:A:213:ASN:ND2	1:A:237:HIS:HA	2.32	0.44
1:A:279:ILE:HG13	1:A:280:ALA:H	1.81	0.44
1:A:836:ARG:NH2	3:T:4:DT:H73	2.32	0.44
1:A:1119:LYS:O	1:A:1123:LEU:HD12	2.17	0.44
1:B:649:MET:HE3	1:B:846:MET:HE1	1.98	0.44
1:B:1016:TYR:HA	1:B:1019:VAL:CG2	2.47	0.44
1:A:681:LEU:HB2	1:A:849:ILE:HD13	1.99	0.44
1:B:655:GLN:HG3	1:B:658:SER:HB2	1.98	0.44
1:B:607:VAL:HG23	1:B:895:LEU:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:ARG:HB2	1:B:755:ILE:HG12	1.99	0.44
1:B:965:ILE:HD11	1:B:968:ARG:HD3	1.99	0.44
1:A:1112:PHE:CG	1:A:1137:ILE:HD11	2.53	0.44
1:B:876:THR:HB	2:C:11:DOC:H3'2	2.00	0.43
1:B:981:LEU:HD21	1:B:986:LEU:HD23	2.00	0.43
1:A:836:ARG:HB2	3:T:5:DT:H4'	2.00	0.43
1:B:610:PHE:O	1:B:613:ILE:CG1	2.63	0.43
1:A:645:TYR:CG	4:A:1301:DTP:H2'1	2.53	0.43
1:A:969:TYR:CE2	1:A:982:LYS:HG3	2.53	0.43
1:B:836:ARG:HH22	3:D:4:DT:H72	1.83	0.43
1:B:928:ASP:HB3	1:B:933:ILE:HB	2.01	0.43
1:A:1019:VAL:HG12	1:A:1158:ILE:HG12	1.99	0.43
1:B:50:MET:HE3	1:B:370:ARG:HA	2.00	0.43
1:B:607:VAL:HG21	1:B:893:PHE:HB3	2.00	0.43
1:A:1076:PHE:CD1	1:A:1076:PHE:O	2.70	0.43
1:A:500:ILE:HD13	1:A:515:LEU:HD22	2.01	0.43
1:B:47:ASP:OD2	1:B:130:LYS:NZ	2.50	0.43
1:B:342:GLU:CD	1:B:342:GLU:H	2.27	0.43
1:B:845:GLU:O	1:B:849:ILE:HG12	2.19	0.43
1:A:360:GLN:HE21	1:A:396:LEU:HD21	1.83	0.43
1:B:338:THR:HG23	1:B:344:PRO:HA	2.00	0.43
1:B:781:ARG:NH2	1:B:820:GLN:OE1	2.44	0.43
1:A:332:ILE:HG23	1:A:349:ILE:HG21	2.01	0.43
1:A:858:ILE:HD12	1:A:858:ILE:HA	1.88	0.43
1:A:875:ASP:CG	2:P:11:DOC:H4'	2.43	0.43
1:A:978:LEU:HD21	1:A:981:LEU:HB2	2.00	0.43
1:B:349:ILE:N	1:B:349:ILE:CD1	2.81	0.43
1:B:1097:PRO:HG3	1:B:1128:LEU:HB2	2.01	0.42
1:A:76:VAL:HG22	1:A:266:LYS:HB2	2.01	0.42
1:A:630:ARG:HD3	1:A:632:GLU:OE2	2.19	0.42
1:B:584:LEU:HG	1:B:905:TYR:OH	2.19	0.42
1:B:887:PHE:CG	1:B:888:PRO:HD2	2.55	0.42
1:B:1169:ASN:HD22	1:B:1171:VAL:H	1.59	0.42
1:A:623:GLU:CD	1:A:630:ARG:HH22	2.28	0.42
1:A:328:ILE:HD12	1:A:328:ILE:N	2.34	0.42
1:A:655:GLN:OE1	1:A:771:VAL:HG23	2.19	0.42
1:A:1076:PHE:CD2	1:A:1077:LEU:HG	2.55	0.42
1:B:592:LEU:O	1:B:596:VAL:HG23	2.20	0.42
1:A:891:TYR:HB2	1:A:903:LEU:HD23	2.00	0.42
1:A:1042:LEU:HD11	1:A:1143:TRP:HH2	1.84	0.42
1:B:153:GLU:OE1	1:B:169:ILE:HD11	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:567:ARG:NH2	1:B:1015:CYS:HB2	2.35	0.42
1:B:1141:ILE:HG23	1:B:1146:TYR:CE2	2.55	0.42
1:A:985:GLU:O	1:A:996:LYS:NZ	2.50	0.42
1:B:148:ARG:HB2	1:B:151:ASP:HB2	2.01	0.42
1:B:373:VAL:HG11	1:B:485:TYR:CZ	2.54	0.42
1:A:288:ALA:HA	1:A:375:SER:O	2.20	0.42
1:B:386:PHE:O	1:B:390:ARG:HG2	2.20	0.42
1:B:472:GLU:HA	1:B:475:VAL:CG2	2.50	0.42
1:B:609:ASN:HB2	1:B:612:GLU:CD	2.45	0.42
1:B:754:GLU:HG3	1:B:755:ILE:N	2.35	0.42
1:A:1040:GLU:CD	1:A:1040:GLU:H	2.28	0.41
1:B:870:ARG:HB2	1:B:882:ILE:HG13	2.02	0.41
1:B:1137:ILE:CG2	1:B:1141:ILE:HD11	2.50	0.41
1:B:82:MET:HE3	1:B:82:MET:HB2	1.88	0.41
1:A:968:ARG:HA	1:A:982:LYS:O	2.20	0.41
1:B:613:ILE:HD12	1:B:614:LYS:CA	2.42	0.41
1:A:455:ASP:OD2	1:A:456:PRO:N	2.53	0.41
3:T:15:DT:H2"	3:T:16:DA:C8	2.55	0.41
1:B:915:HIS:HA	1:B:940:ASN:ND2	2.35	0.41
1:A:349:ILE:HD12	1:A:349:ILE:N	2.36	0.41
1:A:834:VAL:HG21	1:A:846:MET:HE2	2.02	0.41
1:B:170:ILE:HD12	1:B:170:ILE:C	2.45	0.41
1:B:1011:THR:HG23	1:B:1014:GLY:N	2.23	0.41
1:B:1112:PHE:CD1	1:B:1137:ILE:CD1	2.99	0.41
1:B:959:LYS:O	1:B:1179:TRP:NE1	2.47	0.41
1:A:747:TYR:C	1:A:749:ARG:H	2.28	0.41
1:B:143:CYS:SG	1:B:152:VAL:HG11	2.61	0.41
1:B:310:MET:HB3	1:B:321:LEU:HD11	2.02	0.41
1:B:607:VAL:CG2	1:B:895:LEU:HB3	2.41	0.41
1:B:787:LEU:HD13	1:B:816:TYR:CZ	2.56	0.41
1:B:1094:SER:O	1:B:1105:ARG:HD2	2.20	0.41
1:A:458:LEU:C	1:A:461:PRO:HD2	2.45	0.41
1:A:616:GLN:O	1:A:620:LYS:HG3	2.21	0.41
1:B:594:PHE:CE1	1:B:598:VAL:HG21	2.55	0.41
1:B:968:ARG:NH2	1:B:985:GLU:OE2	2.53	0.41
1:A:778:ARG:NH1	1:A:779:ASP:OD1	2.54	0.41
1:A:875:ASP:O	1:A:877:ASP:N	2.54	0.41
1:B:125:GLU:OE1	1:B:125:GLU:CA	2.67	0.41
1:B:487:LYS:HD3	1:B:487:LYS:HA	1.92	0.41
1:B:594:PHE:O	1:B:598:VAL:HG22	2.21	0.41
1:A:309:MET:CE	1:A:460:THR:HA	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1005:VAL:HG13	1:A:1008:GLU:OE1	2.21	0.41
1:A:1124:ARG:NE	1:A:1132:LEU:O	2.42	0.41
1:B:287:MET:HB2	1:B:315:ILE:HG23	2.03	0.41
1:B:374:ILE:HG13	1:B:417:CYS:SG	2.61	0.41
1:A:234:ASP:OD2	1:A:234:ASP:N	2.54	0.40
1:A:314:MET:CE	1:A:479:VAL:HA	2.51	0.40
1:A:1116:ILE:HD12	1:A:1116:ILE:H	1.87	0.40
1:B:468:GLN:O	1:B:468:GLN:HG3	2.20	0.40
1:B:561:LEU:HD12	1:B:871:PRO:HG2	2.03	0.40
1:B:678:ALA:HB1	1:B:761:ILE:CG2	2.52	0.40
1:A:246:ASP:OD1	1:A:246:ASP:N	2.54	0.40
1:B:310:MET:CE	1:B:470:LEU:HG	2.51	0.40
1:B:335:PHE:HE2	1:B:475:VAL:HG21	1.86	0.40
1:B:864:LEU:O	1:B:868:VAL:HG23	2.21	0.40
1:A:964:GLY:O	1:A:965:ILE:HD13	2.20	0.40
1:A:696:GLU:HG2	1:A:742:TYR:OH	2.21	0.40
1:B:310:MET:HE3	1:B:474:SER:OG	2.22	0.40
1:B:889:GLU:HB3	1:B:890:THR:H	1.80	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1093/1191 (92%)	1043 (95%)	47 (4%)	3 (0%)	36	55
1	B	1087/1191 (91%)	1031 (95%)	52 (5%)	4 (0%)	30	49
All	All	2180/2382 (92%)	2074 (95%)	99 (4%)	7 (0%)	36	55

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	710	PRO
1	A	876	THR
1	B	876	THR
1	A	1119	LYS
1	B	279	ILE
1	A	990	GLY
1	B	218	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	921/1066 (86%)	921 (100%)	0	100	100
1	B	883/1066 (83%)	883 (100%)	0	100	100
All	All	1804/2132 (85%)	1804 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	A	324	ASN
1	A	360	GLN
1	A	389	ASN
1	A	993	GLN
1	B	36	GLN
1	B	83	HIS
1	B	111	ASN
1	B	197	ASN
1	B	198	GLN
1	B	269	GLN
1	B	307	GLN
1	B	523	GLN
1	B	546	HIS
1	B	586	GLN

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Mol	Chain	Res	Type
1	B	631	ASN
1	B	859	GLN
1	B	922	GLN
1	B	924	GLN
1	B	940	ASN
1	B	1088	GLN
1	B	1169	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	C	11	2,3	16,19,20	2.58	4 (25%)	20,26,29	1.67	4 (20%)
2	DOC	P	11	2,3	16,19,20	2.56	4 (25%)	20,26,29	1.87	3 (15%)

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	C	11	2,3	-	3/7/18/19	0/2/2/2
2	DOC	P	11	2,3	-	3/7/18/19	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	DOC	C6-C5	7.97	1.53	1.35
2	P	11	DOC	C6-C5	7.96	1.53	1.35
2	C	11	DOC	C6-N1	4.26	1.48	1.38
2	P	11	DOC	C6-N1	4.25	1.48	1.38
2	C	11	DOC	C2-N1	-3.25	1.33	1.40
2	P	11	DOC	C2-N1	-3.14	1.33	1.40
2	C	11	DOC	C4-N3	2.50	1.39	1.34
2	P	11	DOC	C4-N3	2.28	1.39	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	11	DOC	C4'-O4'-C1'	-5.24	104.86	109.81
2	C	11	DOC	C5-C4-N4	-3.32	114.82	120.63
2	C	11	DOC	C5-C6-N1	-3.27	116.53	121.84
2	P	11	DOC	C5-C4-N4	-3.21	115.02	120.63
2	P	11	DOC	C5-C6-N1	-3.19	116.65	121.84
2	C	11	DOC	O4'-C1'-N1	-2.11	104.11	107.86
2	C	11	DOC	C4'-O4'-C1'	-2.11	107.81	109.81

There are no chirality outliers.

All (6) 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
2	P	11	DOC	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 7 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	B	1301	5	31,32,32	1.65	7 (22%)	46,50,50	1.95	11 (23%)
4	DTP	A	1301	5	31,32,32	1.66	7 (22%)	46,50,50	1.98	12 (26%)

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	B	1301	5	-	4/22/34/34	0/3/3/3
4	DTP	A	1301	5	-	7/22/34/34	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	DTP	C5-N7	-3.35	1.33	1.39
4	A	1301	DTP	C5-N7	-3.31	1.33	1.39
4	B	1301	DTP	C5-C4	-3.29	1.33	1.39
4	A	1301	DTP	C5-C4	-3.28	1.33	1.39
4	A	1301	DTP	C2-N1	3.13	1.39	1.33
4	B	1301	DTP	C2-N3	3.07	1.39	1.33
4	A	1301	DTP	C2-N3	3.06	1.39	1.33
4	B	1301	DTP	C2-N1	2.97	1.39	1.33
4	B	1301	DTP	C5-C6	-2.90	1.32	1.41
4	A	1301	DTP	C5-C6	-2.83	1.33	1.41
4	A	1301	DTP	C8-N9	-2.78	1.32	1.37
4	B	1301	DTP	C8-N9	-2.76	1.32	1.37
4	A	1301	DTP	C4-N9	-2.43	1.32	1.37
4	B	1301	DTP	C4-N9	-2.32	1.32	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DTP	N3-C2-N1	-6.99	118.00	128.58
4	B	1301	DTP	N3-C2-N1	-6.85	118.22	128.58
4	B	1301	DTP	N9-C8-N7	-4.41	107.68	113.94
4	A	1301	DTP	N9-C8-N7	-4.36	107.76	113.94
4	B	1301	DTP	C5-C4-N3	-4.33	120.75	126.72
4	A	1301	DTP	C5-C4-N3	-4.26	120.85	126.72
4	A	1301	DTP	C2-N3-C4	3.25	119.76	111.83
4	B	1301	DTP	C2-N3-C4	3.20	119.66	111.83
4	B	1301	DTP	C5-N7-C8	3.03	108.21	103.45
4	A	1301	DTP	C5-N7-C8	2.98	108.13	103.45
4	B	1301	DTP	C5-C6-N6	-2.87	116.18	123.29
4	A	1301	DTP	C5-C6-N6	-2.77	116.43	123.29
4	B	1301	DTP	C6-C5-C4	2.58	120.71	117.18
4	B	1301	DTP	C4-N9-C8	2.58	108.45	105.74
4	B	1301	DTP	N3-C4-N9	2.57	131.54	127.17
4	A	1301	DTP	C4-N9-C8	2.51	108.38	105.74
4	A	1301	DTP	C6-C5-C4	2.51	120.60	117.18
4	A	1301	DTP	N3-C4-N9	2.40	131.26	127.17
4	A	1301	DTP	C4-C5-N7	-2.39	107.85	110.58
4	B	1301	DTP	C4-C5-N7	-2.30	107.95	110.58
4	B	1301	DTP	C2'-C1'-N9	-2.24	109.36	114.63
4	A	1301	DTP	C2'-C1'-N9	-2.10	109.68	114.63
4	A	1301	DTP	O3G-PG-O2G	2.01	115.34	107.80

There are no chirality outliers.

All (11) torsion outliers are listed below:

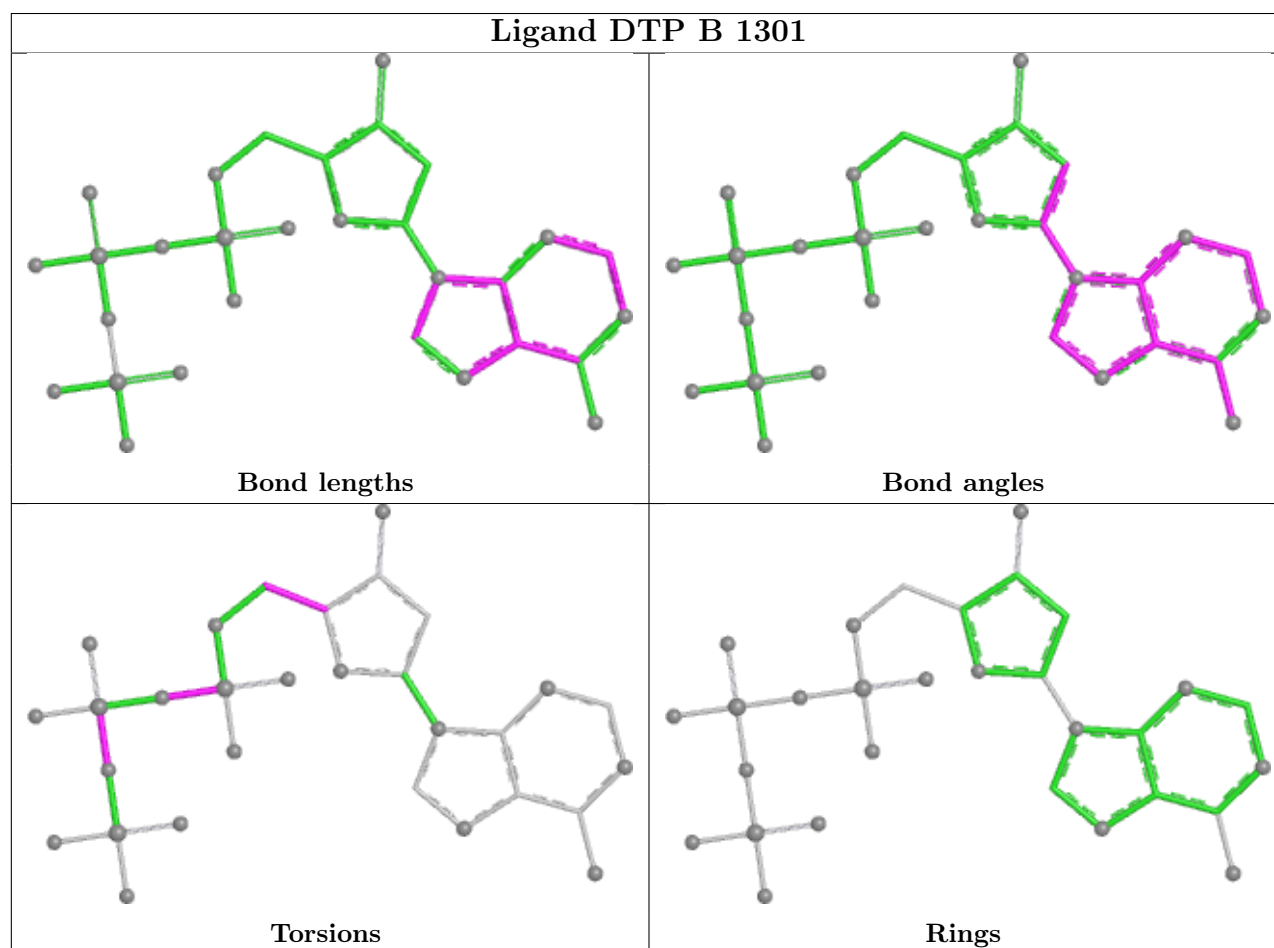
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3A-PA-O1A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	PB-O3A-PA-O1A
4	A	1301	DTP	PG-O3B-PB-O1B
4	A	1301	DTP	PG-O3B-PB-O2B
4	A	1301	DTP	PA-O3A-PB-O1B
4	A	1301	DTP	PB-O3A-PA-O2A
4	B	1301	DTP	O4'-C4'-C5'-O5'
4	A	1301	DTP	PA-O3A-PB-O2B
4	B	1301	DTP	PB-O3A-PA-O2A
4	B	1301	DTP	PG-O3B-PB-O2B

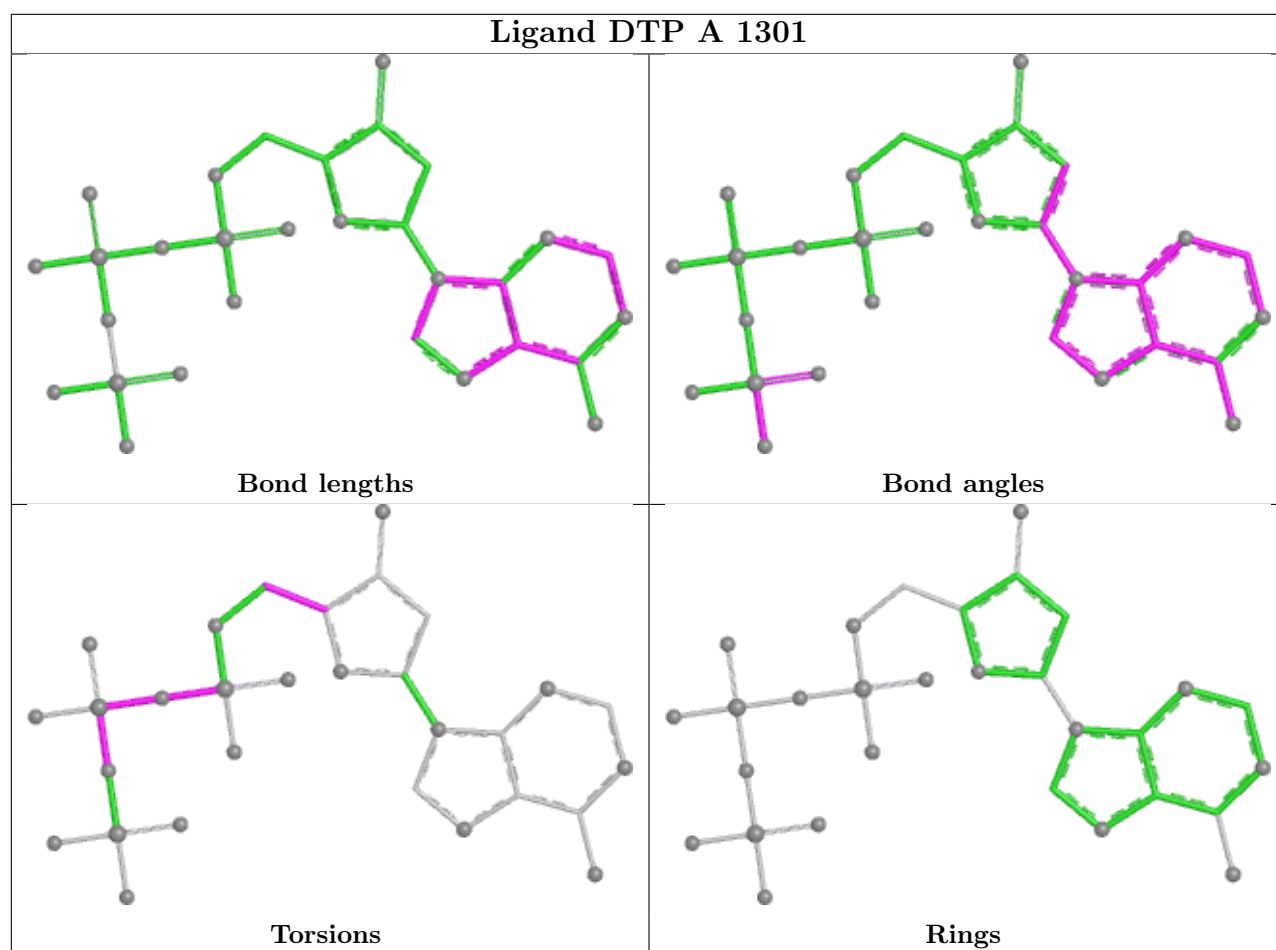
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1301	DTP	2	0
4	A	1301	DTP	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	1103/1191 (92%)	0.40	40 (3%)	46	41	46, 72, 97, 119	0
1	B	1099/1191 (92%)	0.55	65 (5%)	28	24	44, 75, 102, 118	0
2	C	10/11 (90%)	-0.04	0	100	100	52, 64, 73, 81	1 (10%)
2	P	10/11 (90%)	-0.20	0	100	100	49, 62, 70, 75	1 (10%)
3	D	15/15 (100%)	0.06	0	100	100	48, 61, 82, 100	0
3	T	15/15 (100%)	-0.17	0	100	100	47, 59, 83, 101	0
All	All	2252/2434 (92%)	0.47	105 (4%)	36	32	44, 73, 100, 119	2 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	690	PHE	4.9
1	B	692	SER	4.8
1	B	30	TYR	4.6
1	B	743	SER	4.3
1	B	691	PRO	4.2
1	B	217	ASN	4.2
1	A	720	VAL	3.9
1	A	750	VAL	3.7
1	B	1185	ALA	3.6
1	B	704	LEU	3.6
1	B	676	THR	3.6
1	B	742	TYR	3.5
1	B	596	VAL	3.4
1	B	740	THR	3.4
1	A	308	ILE	3.4
1	A	547	LEU	3.1
1	B	604	VAL	3.1
1	A	722	THR	3.1
1	B	328	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	31	ALA	3.1
1	A	702	ARG	3.1
1	A	693	LYS	3.0
1	A	706	ASN	3.0
1	B	901	LEU	2.9
1	A	697	TYR	2.9
1	A	748	HIS	2.8
1	B	613	ILE	2.8
1	B	894	THR	2.8
1	A	64	PHE	2.8
1	B	589	PRO	2.7
1	B	216	ASN	2.7
1	B	310	MET	2.7
1	B	608	THR	2.6
1	B	734	HIS	2.6
1	A	1046	ILE	2.6
1	B	1184	ILE	2.5
1	A	470	LEU	2.5
1	B	1050	ARG	2.5
1	A	624	LEU	2.5
1	A	1185	ALA	2.5
1	B	697	TYR	2.4
1	B	323	THR	2.4
1	A	990	GLY	2.4
1	A	328	ILE	2.4
1	A	1128	LEU	2.4
1	B	902	TYR	2.4
1	B	722	THR	2.4
1	B	896	GLU	2.4
1	B	990	GLY	2.4
1	B	897	ASN	2.4
1	A	1064	SER	2.3
1	A	219	GLN	2.3
1	A	704	LEU	2.3
1	B	699	MET	2.3
1	B	895	LEU	2.3
1	B	694	MET	2.3
1	A	723	PHE	2.3
1	A	1019	VAL	2.3
1	B	598	VAL	2.3
1	B	615	ASN	2.3
1	A	705	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	624	LEU	2.3
1	B	1140	ILE	2.3
1	A	899	LYS	2.3
1	B	732	VAL	2.3
1	B	287	MET	2.3
1	A	234	ASP	2.2
1	B	467	PRO	2.2
1	A	747	TYR	2.2
1	A	708	THR	2.2
1	A	1076	PHE	2.2
1	B	700	ILE	2.2
1	A	1079	GLU	2.2
1	A	691	PRO	2.2
1	A	298	LEU	2.2
1	B	588	LEU	2.2
1	B	464	PHE	2.2
1	B	219	GLN	2.1
1	A	1034	GLY	2.1
1	B	1135	LEU	2.1
1	B	578	PRO	2.1
1	B	224	ASN	2.1
1	B	706	ASN	2.1
1	B	114	ILE	2.1
1	A	896	GLU	2.1
1	A	935	GLU	2.1
1	B	886	SER	2.1
1	B	701	LYS	2.1
1	B	582	ASP	2.1
1	B	580	ALA	2.1
1	A	32	LEU	2.1
1	B	693	LYS	2.1
1	B	602	SER	2.1
1	B	603	SER	2.1
1	B	87	VAL	2.0
1	B	744	ARG	2.0
1	A	721	LEU	2.0
1	B	726	LEU	2.0
1	A	1179	TRP	2.0
1	A	710	PRO	2.0
1	B	756	VAL	2.0
1	B	235	ALA	2.0
1	B	584	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	678	ALA	2.0
1	B	798	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	DOC	C	11	18/19	0.93	0.10	40,53,66,67	0
2	DOC	P	11	18/19	0.96	0.08	40,47,57,59	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

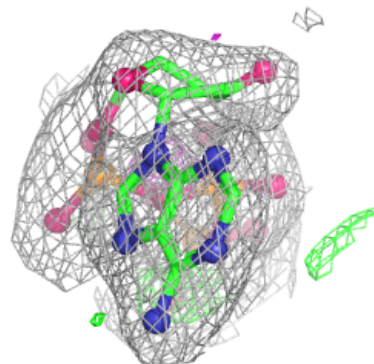
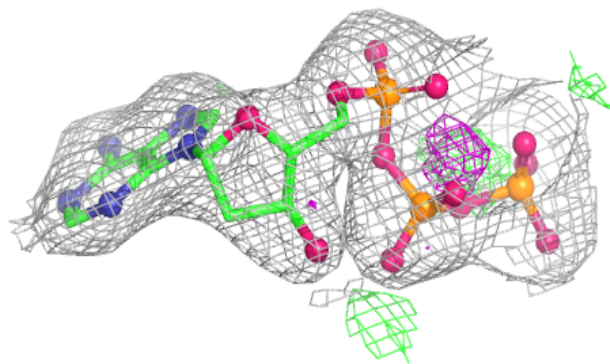
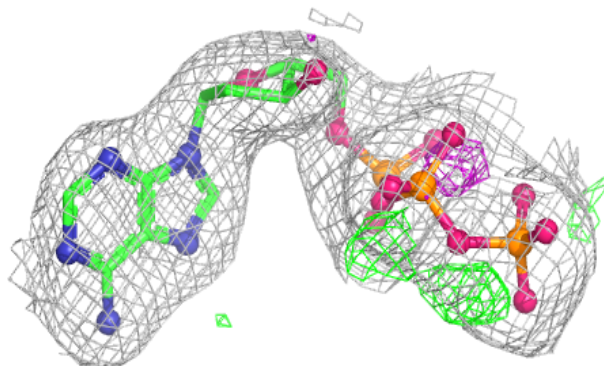
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CA	B	1303	1/1	0.71	0.14	86,86,86,86	1
6	FE	A	1304	1/1	0.77	0.21	102,102,102,102	1
5	CA	B	1304	1/1	0.79	0.11	90,90,90,90	1
6	FE	B	1305	1/1	0.85	0.21	92,92,92,92	1
4	DTP	A	1301	30/30	0.95	0.08	39,50,61,66	0
4	DTP	B	1301	30/30	0.96	0.07	41,50,63,65	0
5	CA	A	1303	1/1	0.97	0.08	82,82,82,82	1
5	CA	B	1302	1/1	0.97	0.04	58,58,58,58	0
5	CA	A	1302	1/1	0.98	0.05	60,60,60,60	0

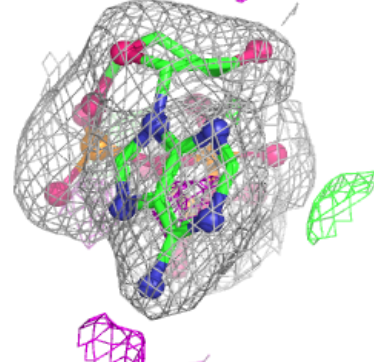
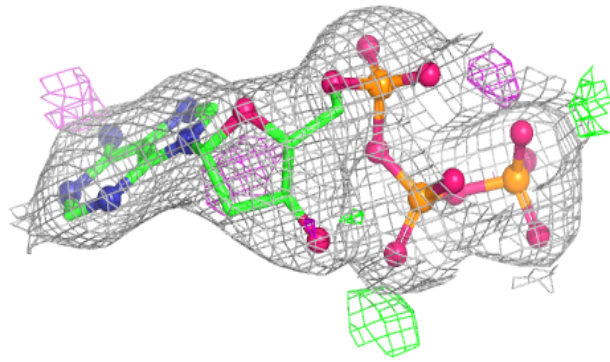
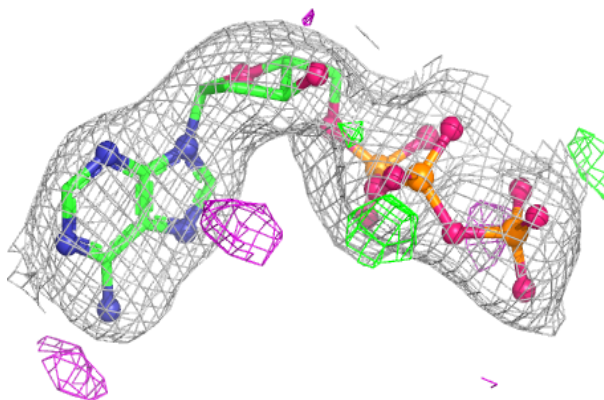
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DTP B 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.