Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2024 – 04:49 am BST

PDB ID	:	6FWK
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:

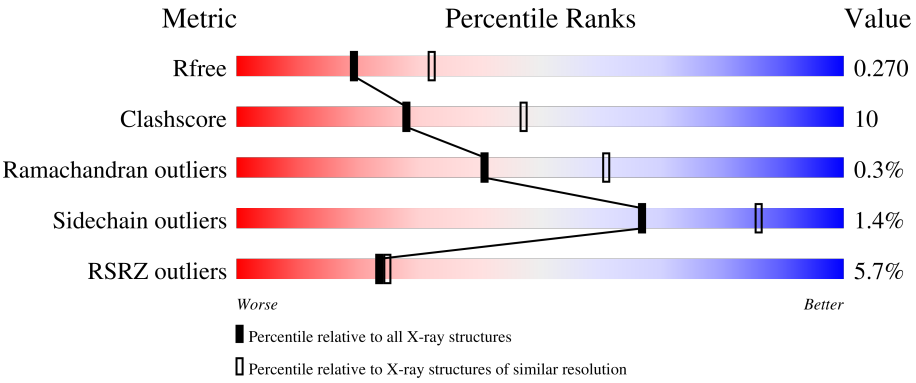
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	5% 77% 15% 7%
1	B	1191	6% 72% 19% 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	

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

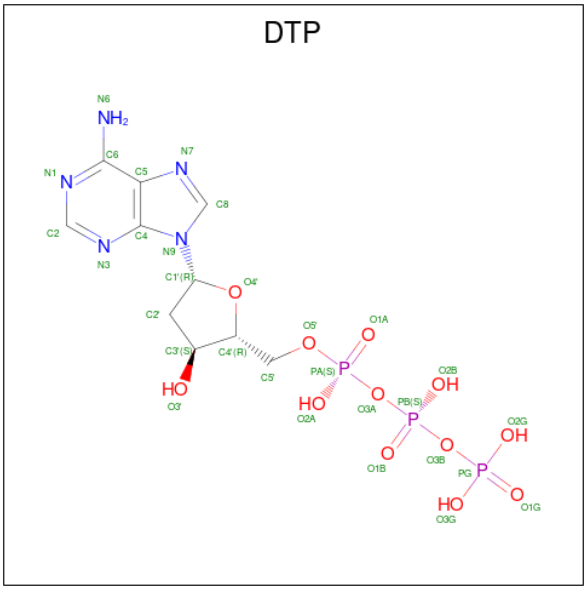
- Molecule 2 is a DNA chain called DNA (5'-D(P*TP*AP*AP*CP*CP*GP*CP*GP*TP*TP *(DOC))-3').

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 (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	A	2	Total	Ca	0	0
			2	2		
5	B	3	Total	Ca	0	0
			3	3		

- Molecule 6 is FE (III) ION (three-letter code: 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 Fe 1 1	0	0

- Molecule 7 is water.

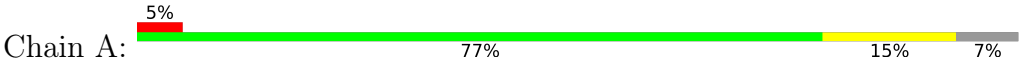
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	5	Total O 5 5	0	0
7	B	6	Total O 6 6	0	0

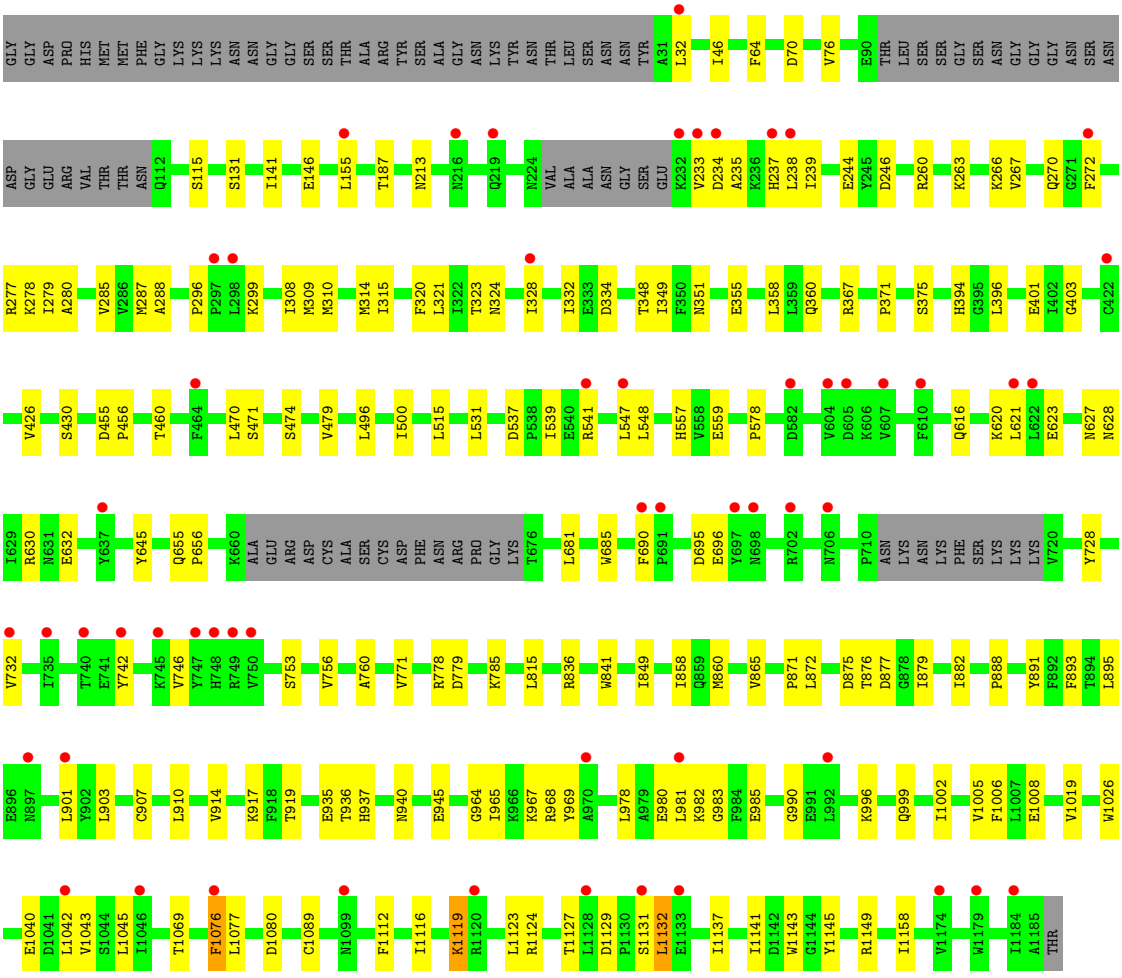
3 Residue-property plots (i)

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

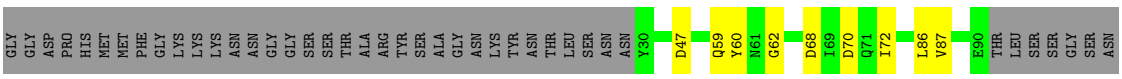
Chain A:

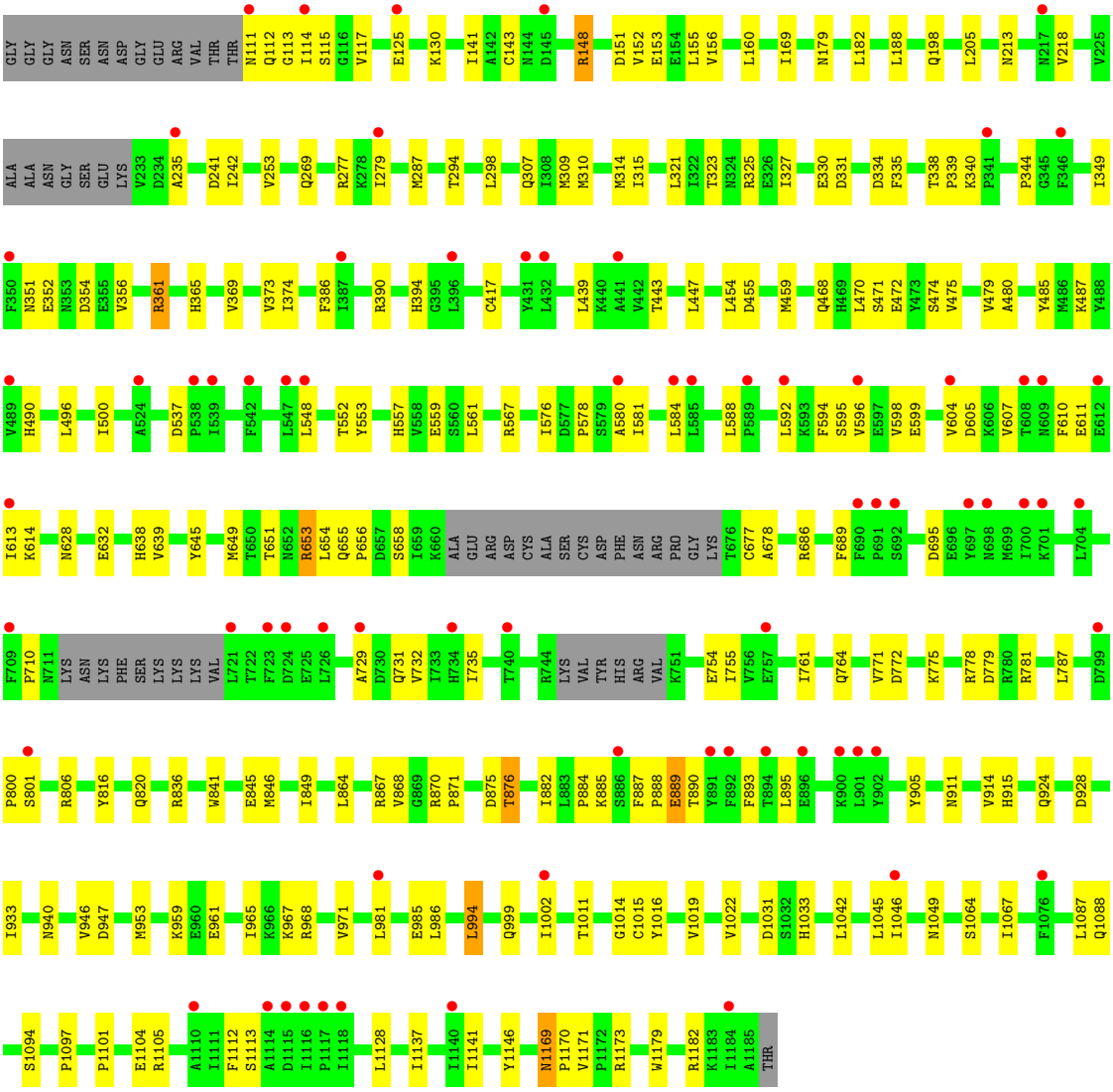




• Molecule 1: DNA polymerase epsilon catalytic subunit A

Chain B:





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

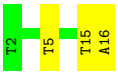
Chain P:

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

Chain C:

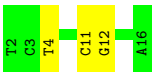
• Molecule 3: DNA (5'-D(P*TP*CP*TP*TP*GP*AP*AP*CP*GP*CP*GP*GP*TP*TP*A)-3'
)

Chain T:



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

Chain D:



4 Data and refinement statistics (i)

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 49.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.99-2.50) 99.3 (49.95-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.263 0.231 , 0.270	Depositor DCC
R_{free} test set	5420 reflections (5.02%)	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)	0.30 , 46.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DOC, CA, FE, DTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.26	0/8929	0.44	0/12114
1	B	0.27	0/8762	0.46	0/11899
2	C	0.53	0/226	0.87	0/346
2	P	0.47	0/226	0.79	0/346
3	D	0.46	0/344	0.93	0/529
3	T	0.48	0/344	0.82	0/529
All	All	0.29	0/18831	0.49	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

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	136	0
1	B	8566	0	8085	210	0
2	C	221	0	125	4	0
2	P	221	0	125	0	0
3	D	308	0	171	2	0
3	T	308	0	171	2	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	349	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 10.

All (349) 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: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:86:LEU:HD23	1:B:114:ILE:C	2.07	0.75
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: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:309:MET:HE3	1:A:460:THR:HA	1.71	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: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:86:LEU:HD22	1:B:113:GLY:C	2.11	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:285:VAL:HG13	1:A:371:PRO:HA	1.76	0.68
1:B:86:LEU:CD2	1:B:114:ILE:C	2.62	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: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: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:B:613:ILE:HD12	1:B:613:ILE:C	2.19	0.63
1:A:155:LEU:HD12	1:A:235:ALA:HB3	1.81	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1112:PHE:CD2	1:B:1137:ILE:HD11	2.35	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: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: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:A:310:MET:HE2	1:A:321:LEU:HD11	1.84	0.58
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: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:607:VAL:HA	1:B:895:LEU:HA	1.87	0.57
1:A:155:LEU:HD23	1:A:155:LEU:C	2.25	0.56
1:A:621:LEU:CD1	1:A:888:PRO:HG2	2.36	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:1169:ASN:HD22	1:B:1169:ASN:C	2.10	0.55
1:B:152:VAL:O	1:B:156:VAL:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:213:ASN:OD1	1:B:213:ASN:C	2.48	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
1:A:324:ASN:HD21	1:A:355:GLU:N	2.08	0.52
1:A:470:LEU:C	1:A:470:LEU:HD23	2.30	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:B:59:GLN:OE1	1:B:269:GLN:NE2	2.44	0.51
1:B:1169:ASN:ND2	1:B:1169:ASN:C	2.64	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:TYR:CZ	1:B:62:GLY:HA3	2.46	0.50
1:B:325:ARG:NH1	1:B:330:GLU:C	2.65	0.50
1:B:198:GLN:HE21	1:B:198:GLN:HA	1.77	0.50
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:155:LEU:C	1:A:155:LEU:CD2	2.81	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
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: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:A:64:PHE:HB2	1:A:270:GLN:CD	2.34	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:A:234:ASP:OD2	1:A:237:HIS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:485:TYR:CE2	1:B:490:HIS:HB2	2.50	0.47
1:B:911:ASN:HA	1:B:914:VAL:CG2	2.43	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:B:294:THR:HA	1:B:309:MET:HE3	1.97	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
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: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:875:ASP:CG	2:C:11:DOC:H4'	2.36	0.45
1:B:325:ARG:HH12	1:B:330:GLU:CA	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:455:ASP:OD2	1:A:455:ASP:C	2.55	0.45
1:B:649:MET:HA	1:B:654:LEU:HD12	1.97	0.45
1:B:314:MET:HE1	1:B:479:VAL:HA	1.99	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: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:1119:LYS:O	1:A:1123:LEU:HD12	2.17	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
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:A:70:ASP:CG	1:A:277:ARG:HH12	2.20	0.43
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:607:VAL:HG21	1:B:893:PHE:HB3	2.00	0.43
1:B:125:GLU:OE1	1:B:125:GLU:CA	2.67	0.43
1:B:454:LEU:HD23	1:B:454:LEU:C	2.38	0.43
1:B:655:GLN:HA	1:B:846:MET:HE2	1.99	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:845:GLU:O	1:B:849:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:70:ASP:CG	1:B:277:ARG:HH12	2.22	0.42
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:935:GLU:OE1	1:A:935:GLU:C	2.58	0.42
1:A:630:ARG:HD3	1:A:632:GLU:OE2	2.19	0.42
1:B:111:ASN:CG	1:B:112:GLN:N	2.73	0.42
1:A:935:GLU:OE1	1:A:936:THR:C	2.58	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: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
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:754:GLU:HG3	1:B:755:ILE:N	2.35	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:616:GLN:O	1:A:620:LYS:HG3	2.21	0.41
1:B:310:MET:HE3	1:B:474:SER:OG	2.20	0.41
1:B:594:PHE:CE1	1:B:598:VAL:HG21	2.55	0.41
1:B:613:ILE:C	1:B:613:ILE:CD1	2.86	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: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: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:323:THR:HG1	1:B:351:ASN:HA	1.77	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:454:LEU:HD23	1:B:455:ASP:C	2.41	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:889:GLU:HB3	1:B:890:THR:H	1.80	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	1093/1191 (92%)	1043 (95%)	47 (4%)	3 (0%)	41 61
1	B	1087/1191 (91%)	1031 (95%)	52 (5%)	4 (0%)	34 54
All	All	2180/2382 (92%)	2074 (95%)	99 (4%)	7 (0%)	41 61

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	921/1066 (86%)	910 (99%)	11 (1%)	71 88
1	B	883/1066 (83%)	869 (98%)	14 (2%)	62 84
All	All	1804/2132 (85%)	1779 (99%)	25 (1%)	67 86

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	A	131	SER
1	A	474	SER
1	A	537	ASP
1	A	695	ASP
1	A	753	SER
1	A	815	LEU
1	A	895	LEU
1	A	907	CYS
1	A	1076	PHE
1	A	1132	LEU
1	B	115	SER
1	B	148	ARG
1	B	188	LEU
1	B	361	ARG
1	B	537	ASP
1	B	653	ARG
1	B	677	CYS
1	B	695	ASP
1	B	801	SER
1	B	889	GLU
1	B	994	LEU
1	B	1033	HIS
1	B	1087	LEU
1	B	1169	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	324	ASN
1	B	111	ASN
1	B	198	GLN
1	B	269	GLN
1	B	307	GLN
1	B	924	GLN
1	B	1169	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	2,3	16,19,20	2.54	4 (25%)	20,26,29	1.91	4 (20%)
2	DOC	C	11	2,3	16,19,20	2.57	4 (25%)	20,26,29	1.72	5 (25%)

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	2,3	-	3/7/18/19	0/2/2/2
2	DOC	C	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	7.95	1.53	1.35
2	P	11	DOC	C6-C5	7.94	1.53	1.35
2	C	11	DOC	C6-N1	4.25	1.48	1.38
2	P	11	DOC	C6-N1	4.24	1.48	1.38
2	C	11	DOC	C2-N1	-3.10	1.33	1.40
2	P	11	DOC	C2-N1	-2.99	1.33	1.40
2	C	11	DOC	C4-N3	2.46	1.39	1.34
2	P	11	DOC	C4-N3	2.25	1.39	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	11	DOC	C4'-O4'-C1'	-5.24	104.86	109.81
2	C	11	DOC	C5-C4-N4	-3.65	114.82	120.57
2	P	11	DOC	C5-C4-N4	-3.53	115.02	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	11	DOC	C5-C6-N1	-3.15	116.53	121.81
2	P	11	DOC	C5-C6-N1	-3.08	116.65	121.81
2	C	11	DOC	O4'-C1'-C2'	-2.15	104.34	106.67
2	C	11	DOC	C4'-O4'-C1'	-2.11	107.81	109.81
2	C	11	DOC	O4'-C1'-N1	-2.10	104.11	107.86
2	P	11	DOC	O4'-C1'-C2'	-2.04	104.46	106.67

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.

1 monomer is involved in 2 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	26,32,32	1.67	4 (15%)	30,50,50	1.81	5 (16%)
4	DTP	A	1301	5	26,32,32	1.65	4 (15%)	30,50,50	1.79	5 (16%)

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	-	3/18/34/34	0/3/3/3
4	DTP	A	1301	5	-	7/18/34/34	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	DTP	C2-N3	4.52	1.39	1.32
4	A	1301	DTP	C2-N3	4.51	1.39	1.32
4	A	1301	DTP	C2-N1	3.00	1.39	1.33
4	B	1301	DTP	C5-C4	-2.92	1.33	1.40
4	A	1301	DTP	C5-C4	-2.91	1.33	1.40
4	B	1301	DTP	C2-N1	2.85	1.39	1.33
4	B	1301	DTP	C6-C5	-2.79	1.32	1.43
4	A	1301	DTP	C6-C5	-2.74	1.33	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1301	DTP	N3-C2-N1	-6.84	118.00	128.68
4	B	1301	DTP	N3-C2-N1	-6.69	118.22	128.68
4	B	1301	DTP	PB-O3B-PG	-3.04	122.39	132.83
4	B	1301	DTP	C5-C6-N6	-2.74	116.18	120.35
4	A	1301	DTP	PB-O3B-PG	-2.67	123.68	132.83
4	A	1301	DTP	C5-C6-N6	-2.58	116.43	120.35
4	B	1301	DTP	PA-O3A-PB	-2.56	124.05	132.83
4	A	1301	DTP	PA-O3A-PB	-2.50	124.24	132.83
4	B	1301	DTP	C2'-C1'-N9	-2.13	109.36	114.27
4	A	1301	DTP	O3G-PG-O2G	2.02	115.34	107.64

There are no chirality outliers.

All (10) torsion outliers are listed below:

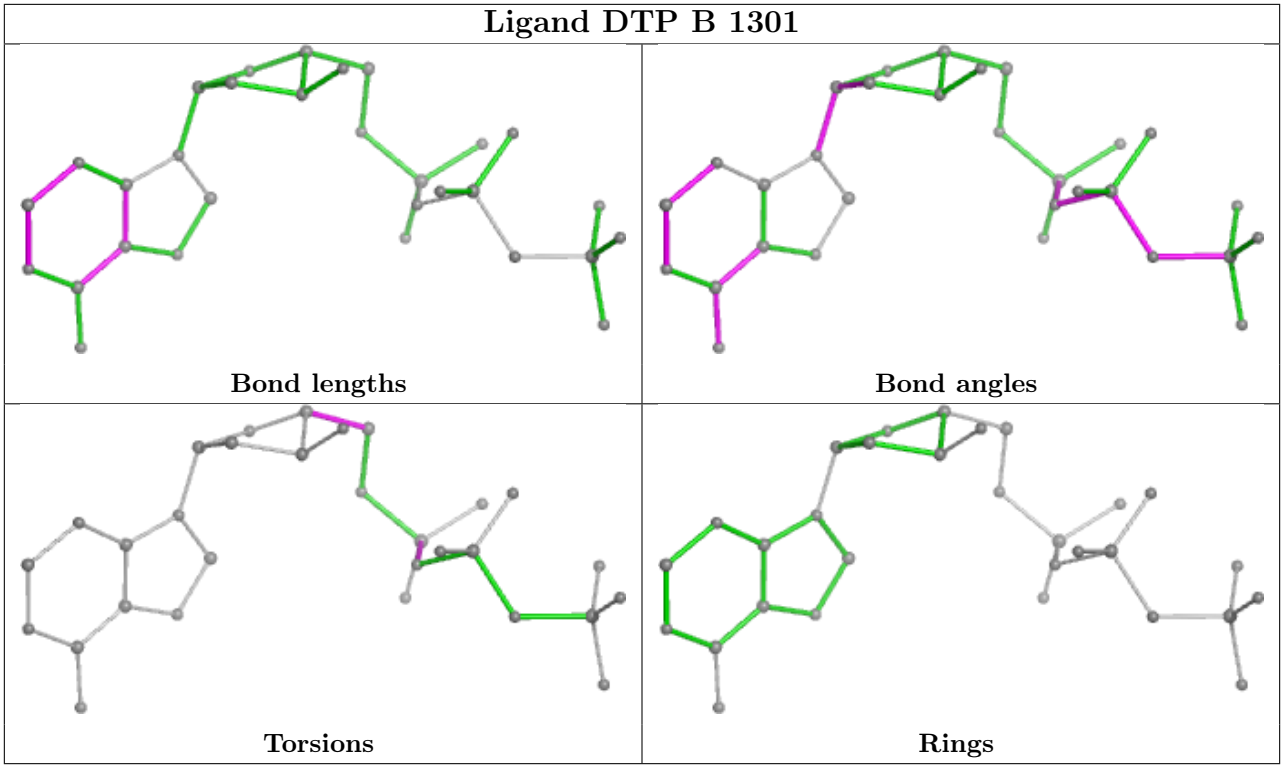
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3A-PA-O1A
4	A	1301	DTP	O4'-C4'-C5'-O5'
4	B	1301	DTP	PB-O3A-PA-O1A
4	A	1301	DTP	PG-O3B-PB-O1B
4	A	1301	DTP	PG-O3B-PB-O2B
4	A	1301	DTP	PA-O3A-PB-O1B
4	A	1301	DTP	PB-O3A-PA-O2A
4	B	1301	DTP	O4'-C4'-C5'-O5'
4	A	1301	DTP	PA-O3A-PB-O2B
4	B	1301	DTP	PB-O3A-PA-O2A

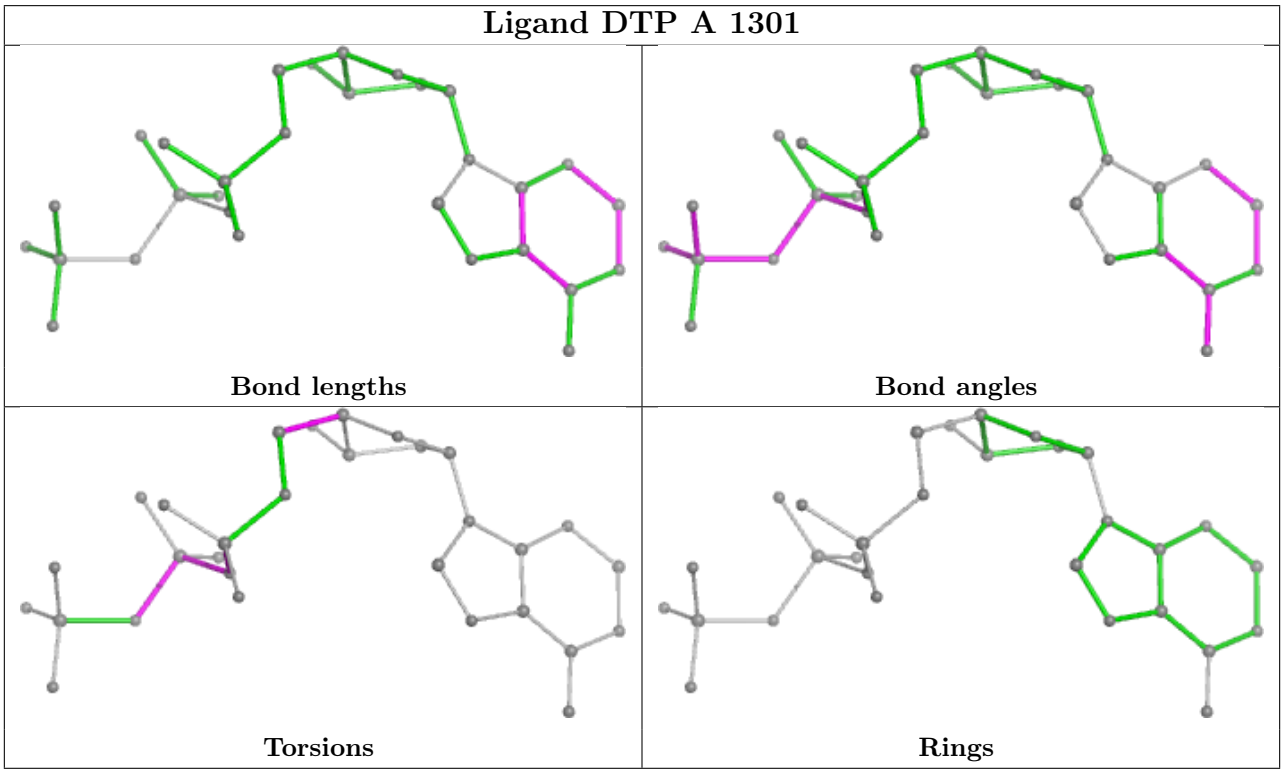
There are no ring outliers.

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.41	56 (5%) 28 29	46, 72, 97, 119	0
1	B	1099/1191 (92%)	0.51	72 (6%) 18 19	44, 75, 102, 118	0
2	C	10/11 (90%)	-0.06	0 100 100	52, 64, 81, 82	1 (10%)
2	P	10/11 (90%)	-0.01	0 100 100	49, 63, 75, 77	1 (10%)
3	D	15/15 (100%)	0.18	0 100 100	48, 61, 82, 100	0
3	T	15/15 (100%)	0.05	0 100 100	47, 59, 83, 101	0
All	All	2252/2434 (92%)	0.45	128 (5%) 23 25	44, 73, 100, 119	2 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	706	ASN	6.1
1	B	894	THR	5.6
1	B	547	LEU	4.8
1	A	464	PHE	4.6
1	B	539	ILE	4.5
1	B	114	ILE	4.4
1	B	801	SER	4.4
1	A	750	VAL	4.3
1	B	729	ALA	4.3
1	B	1118	ILE	4.2
1	A	747	TYR	4.1
1	A	1046	ILE	4.1
1	B	701	LYS	4.1
1	A	234	ASP	3.9
1	B	548	LEU	3.8
1	B	700	ILE	3.8
1	A	547	LEU	3.8
1	A	298	LEU	3.8
1	B	734	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	584	LEU	3.7
1	A	1042	LEU	3.7
1	B	740	THR	3.6
1	A	232	LYS	3.6
1	B	902	TYR	3.6
1	B	697	TYR	3.5
1	A	32	LEU	3.5
1	B	704	LEU	3.4
1	A	610	PHE	3.4
1	A	735	ILE	3.4
1	A	748	HIS	3.4
1	B	580	ALA	3.3
1	A	233	VAL	3.3
1	A	1184	ILE	3.2
1	A	155	LEU	3.2
1	B	608	THR	3.1
1	B	691	PRO	3.0
1	B	613	ILE	3.0
1	B	892	PHE	3.0
1	A	697	TYR	3.0
1	B	592	LEU	2.9
1	B	111	ASN	2.9
1	B	1115	ASP	2.9
1	B	350	PHE	2.9
1	A	238	LEU	2.9
1	A	604	VAL	2.8
1	B	589	PRO	2.8
1	B	1046	ILE	2.8
1	A	749	ARG	2.8
1	B	235	ALA	2.8
1	B	886	SER	2.8
1	A	698	ASN	2.7
1	B	698	ASN	2.7
1	B	585	LEU	2.7
1	B	901	LEU	2.7
1	B	125	GLU	2.7
1	A	1131	SER	2.6
1	A	582	ASP	2.6
1	A	740	THR	2.6
1	A	1174	VAL	2.6
1	B	217	ASN	2.6
1	A	732	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1076	PHE	2.5
1	B	692	SER	2.5
1	A	742	TYR	2.5
1	A	272	PHE	2.5
1	B	1110	ALA	2.5
1	B	612	GLU	2.5
1	B	596	VAL	2.5
1	A	422	CYS	2.4
1	B	757	GLU	2.4
1	B	145	ASP	2.4
1	B	1117	PRO	2.4
1	A	992	LEU	2.4
1	B	524	ALA	2.4
1	A	745	LYS	2.4
1	A	1120	ARG	2.4
1	A	216	ASN	2.4
1	B	609	ASN	2.3
1	A	1099	ASN	2.3
1	A	297	PRO	2.3
1	A	1133	GLU	2.3
1	B	396	LEU	2.3
1	A	607	VAL	2.3
1	B	709	PHE	2.3
1	A	237	HIS	2.3
1	A	702	ARG	2.3
1	A	690	PHE	2.3
1	A	901	LEU	2.3
1	B	1184	ILE	2.2
1	A	1179	TRP	2.2
1	B	723	PHE	2.2
1	B	1116	ILE	2.2
1	B	726	LEU	2.2
1	B	279	ILE	2.2
1	A	622	LEU	2.2
1	B	341	PRO	2.2
1	B	891	TYR	2.2
1	B	799	ASP	2.2
1	A	637	TYR	2.2
1	A	219	GLN	2.2
1	B	489	VAL	2.2
1	B	441	ALA	2.2
1	A	605	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1076	PHE	2.2
1	A	897	ASN	2.1
1	B	1140	ILE	2.1
1	A	621	LEU	2.1
1	A	541	ARG	2.1
1	A	970	ALA	2.1
1	B	387	ILE	2.1
1	B	542	PHE	2.1
1	B	896	GLU	2.1
1	B	346	PHE	2.1
1	B	981	LEU	2.1
1	A	691	PRO	2.1
1	B	1002	ILE	2.1
1	A	1128	LEU	2.1
1	B	1114	ALA	2.0
1	A	328	ILE	2.0
1	B	690	PHE	2.0
1	B	900	LYS	2.0
1	B	538	PRO	2.0
1	A	981	LEU	2.0
1	B	431	TYR	2.0
1	B	604	VAL	2.0
1	B	432	LEU	2.0
1	B	721	LEU	2.0
1	B	724	ASP	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, 95^{th} 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	0.95	0.20	40,53,66,67	0
2	DOC	P	11	18/19	0.96	0.21	40,47,57,59	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

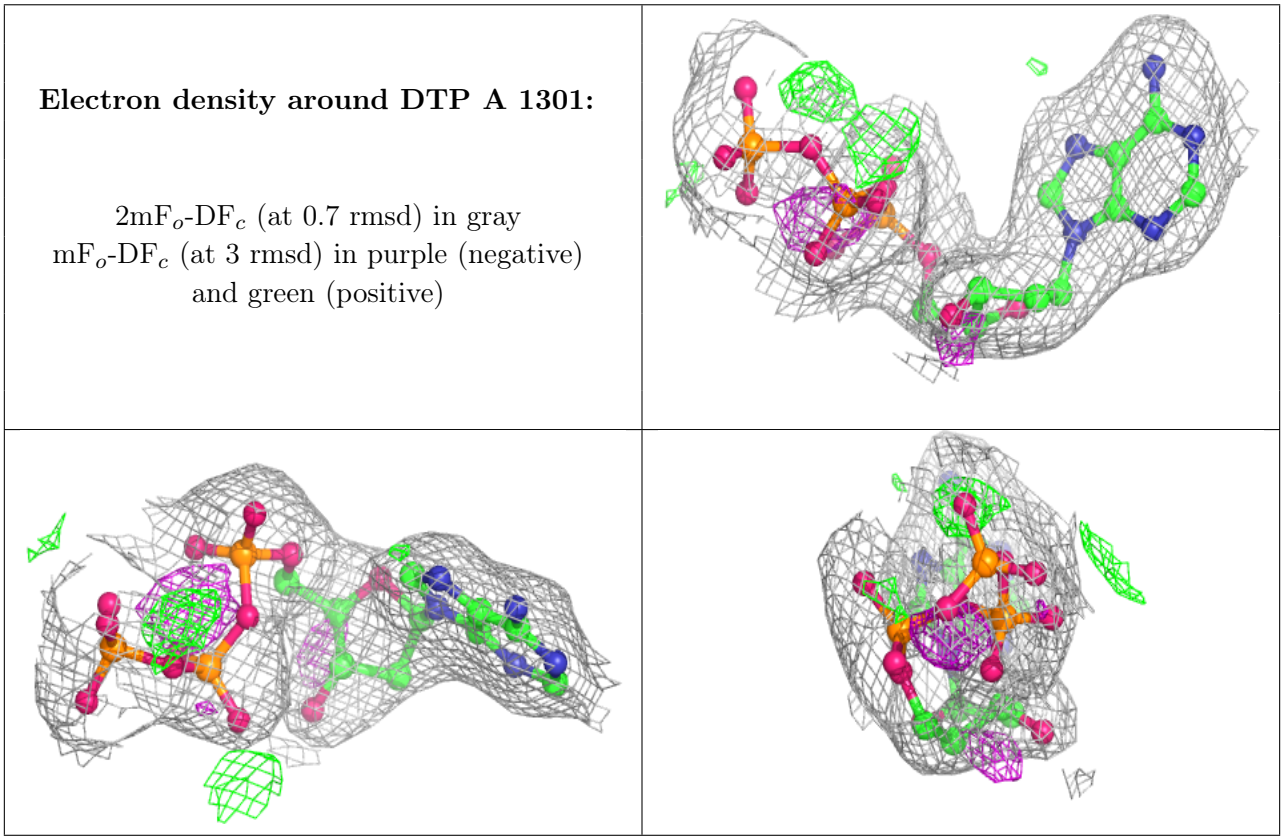
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0.45	0.17	86,86,86,86	1
5	CA	B	1304	1/1	0.45	0.19	90,90,90,90	1
6	FE	A	1304	1/1	0.87	0.26	102,102,102,102	1
4	DTP	A	1301	30/30	0.93	0.17	39,50,61,66	0
5	CA	B	1302	1/1	0.94	0.21	58,58,58,58	0
5	CA	A	1303	1/1	0.94	0.17	82,82,82,82	1
6	FE	B	1305	1/1	0.95	0.30	92,92,92,92	1
5	CA	A	1302	1/1	0.96	0.12	60,60,60,60	0
4	DTP	B	1301	30/30	0.97	0.20	41,50,63,65	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.

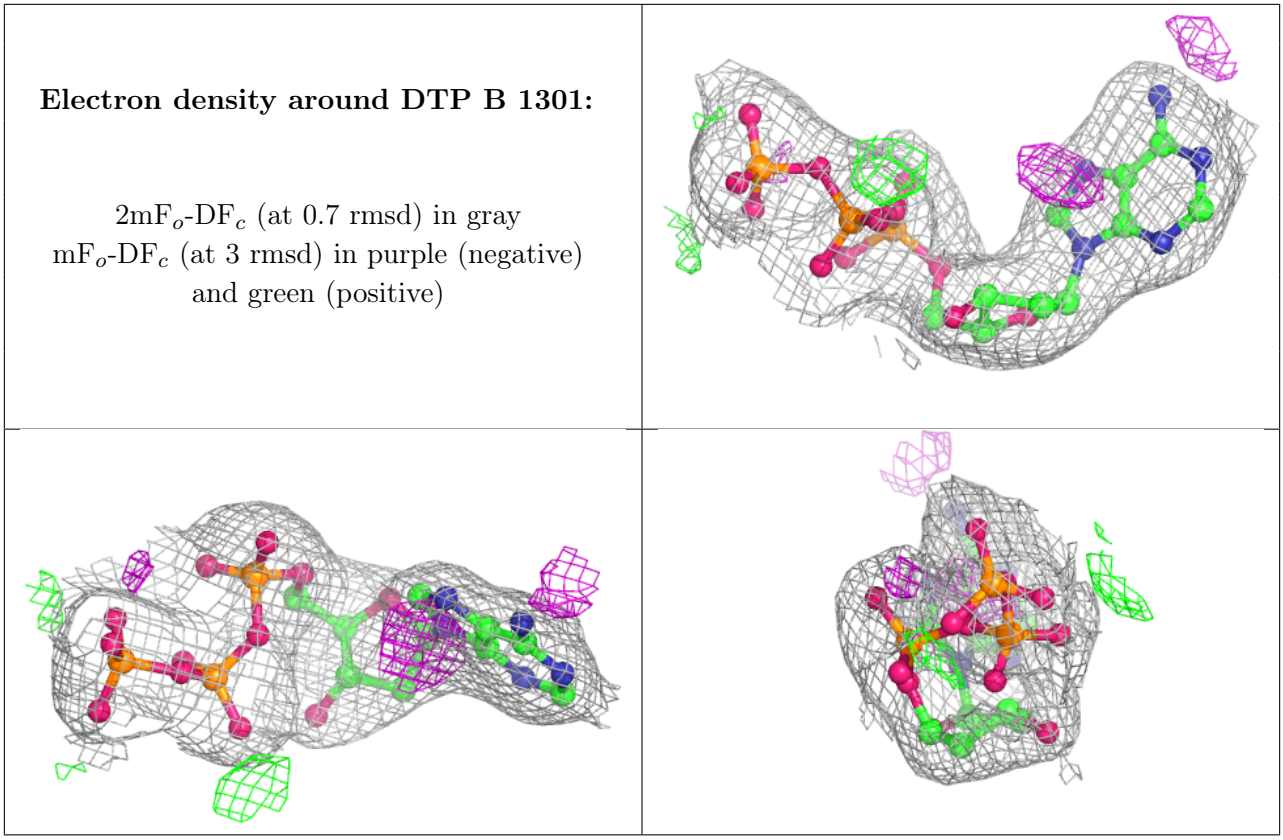
Electron density around DTP A 1301:

$2mF_o$-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.