



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:19 AM UTC

PDB ID : 6I8A / pdb_00006i8a
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 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

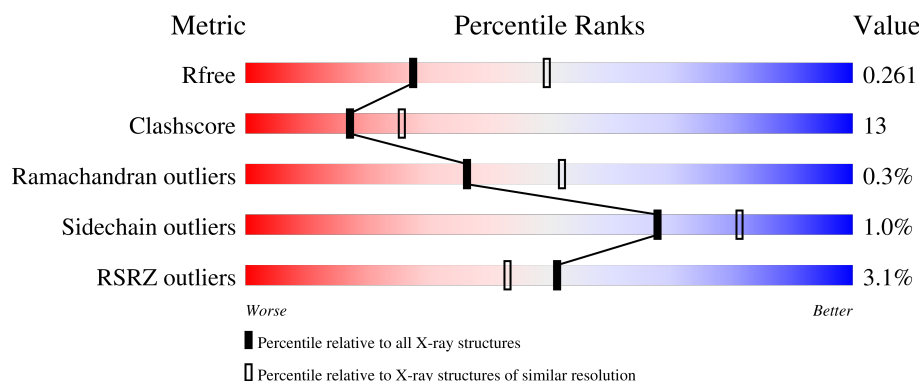
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	1190	
1	B	1190	
2	C	11	
2	P	11	
3	D	16	

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Mol	Chain	Length	Quality of chain
3	T	16	 75%19%6%

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

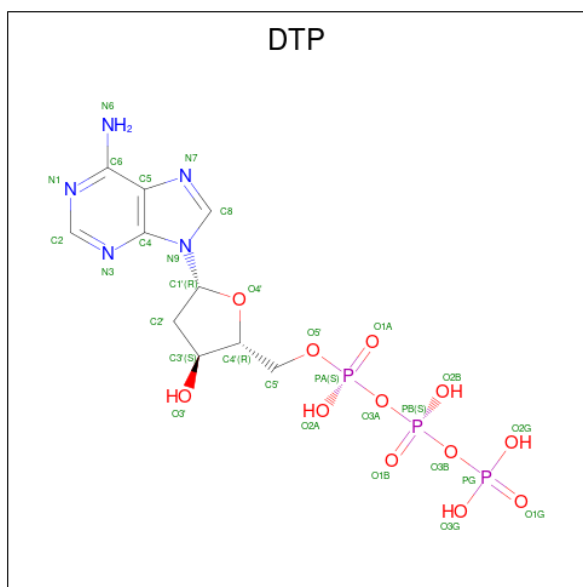
- Molecule 2 is a DNA chain called Primer DNA.

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 (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	2	Total	Ca	0	0
			2	2		

- 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

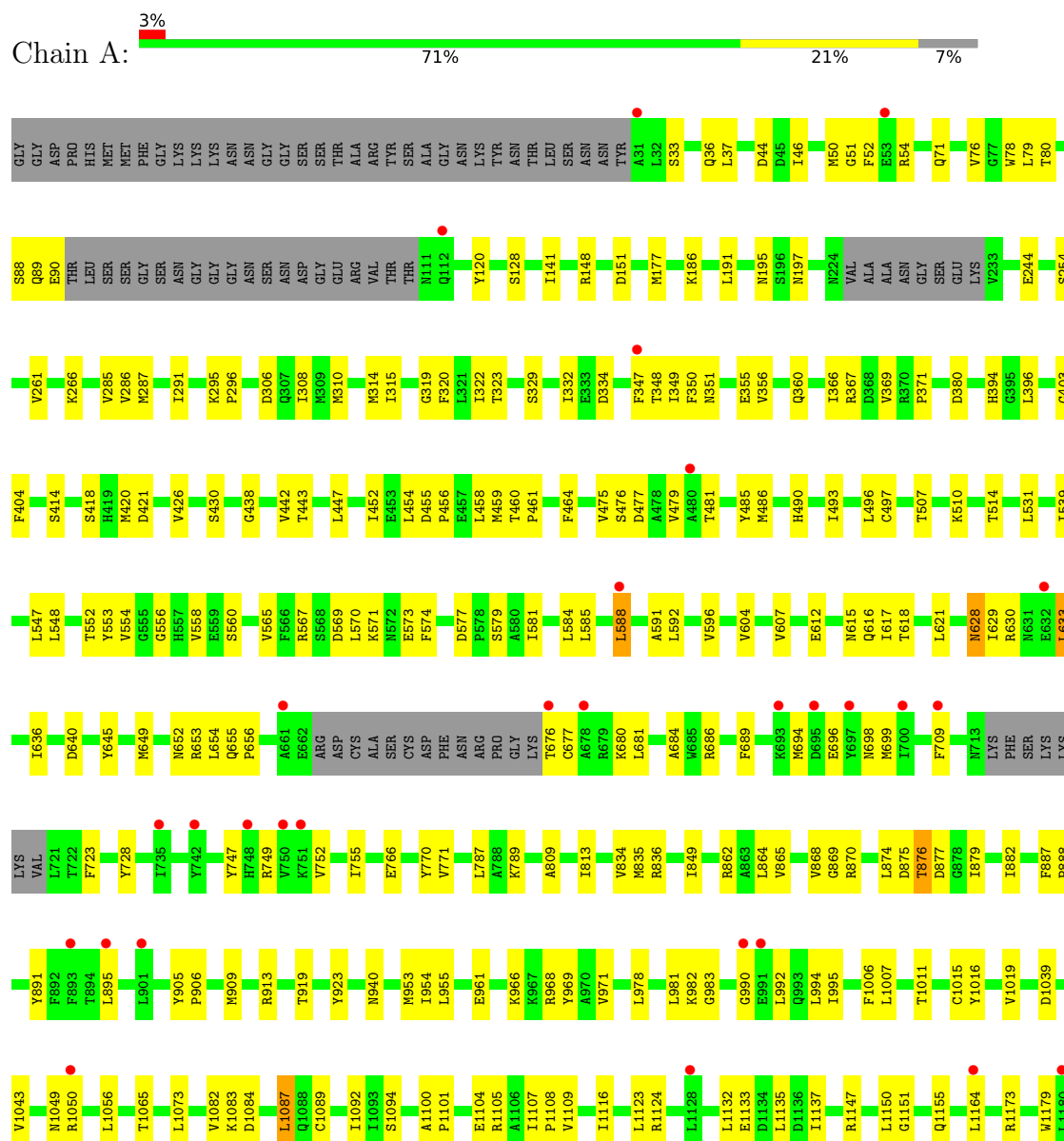
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	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, 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



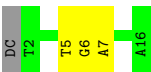




- Molecule 2: Primer DNA



- Molecule 3: Template DNA



- Molecule 3: Template DNA



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 19.96 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.96-2.65) 98.6 (19.96-2.65)	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 (Not available) , 0.261	Depositor DCC
R_{free} test set	4588 reflections (4.99%)	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 , 47.3	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	0.95	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.*

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: DOC, DTP, 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	0.32	0/8768	0.50	4/11921 (0.0%)
1	B	0.38	1/8563 (0.0%)	0.56	11/11657 (0.1%)
2	C	0.36	0/225	0.52	0/344
2	P	0.38	0/225	0.51	0/344
3	D	0.35	0/343	0.47	0/527
3	T	0.36	0/344	0.52	0/529
All	All	0.35	1/18468 (0.0%)	0.53	15/25322 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	827	LEU	CA-C	-5.33	1.45	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	830	PHE	N-CA-C	-9.22	101.23	111.28
1	B	460	THR	CA-C-N	-7.25	111.69	119.24
1	B	460	THR	C-N-CA	-7.25	111.69	119.24
1	A	455	ASP	CA-C-N	6.70	126.21	119.24
1	A	455	ASP	C-N-CA	6.70	126.21	119.24
1	B	831	TYR	N-CA-C	6.68	118.65	111.36
1	B	824	LYS	N-CA-C	6.28	117.79	111.07
1	B	833	TYR	N-CA-C	-5.91	105.92	113.01
1	B	460	THR	N-CA-C	-5.87	104.77	112.75
1	A	633	LEU	CA-C-N	5.66	125.86	120.31
1	A	633	LEU	C-N-CA	5.66	125.86	120.31
1	B	645	TYR	CA-C-N	-5.64	113.38	119.24
1	B	645	TYR	C-N-CA	-5.64	113.38	119.24
1	B	289	PHE	N-CA-C	5.62	117.62	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1119	LYS	N-CA-C	-5.35	105.36	111.14

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	8569	0	8038	184	0
1	B	8369	0	7767	236	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
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	428	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 13.

All (428) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA3	1.48	0.92
1:B:644:MET:HE1	1:B:854:GLY:CA	2.02	0.90
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:A:332:ILE:HG22	1:A:351:ASN:HD21	1.43	0.84
1:B:655:GLN:HA	1:B:846:MET:HE2	1.60	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:994:LEU:HD21	1:B:1150:LEU:HD12	1.65	0.79
1:B:1119:LYS:HB2	1:B:1119:LYS:NZ	1.96	0.79
1:A:287:MET:HE1	1:A:366:ILE:HG12	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
1:A:50:MET:HA	1:A:50:MET:HE2	1.68	0.76
1:B:1138:ARG:HG3	1:B:1138:ARG:NH2	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: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: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:607:VAL:HG21	1:B:893:PHE:HB3	1.74	0.69
1:B:1093:ILE:HD11	1:B:1145:TYR:CD1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:454:LEU:HD11	1:B:459:MET:HG3	1.76	0.63
1:B:1046:ILE:HG23	1:B:1146:TYR:CE2	2.32	0.63
1:B:1112:PHE:CD1	1:B:1137:ILE:HD11	2.32	0.63
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:584:LEU:O	1:A:588:LEU:HD23	2.00	0.62
1:A:585:LEU:HA	1:A:588:LEU:CD2	2.30	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:906:PRO:HA	1:A:909:MET:HE3	1.81	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:A:418:SER:HB3	1:A:420:MET:HE3	1.81	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:A:887:PHE:CE2	1:A:909:MET:HE1	2.36	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:A:310:MET:HE2	1:A:323:THR:HG22	1.82	0.60
1:B:1023:CYS:HB3	1:B:1154:ILE:HD13	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:50:MET:HE1	1:A:367:ARG:O	2.02	0.59
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:N	1:A:71:GLN:OE1	2.35	0.59
1:B:496:LEU:HG	1:B:500:ILE:HD12	1.83	0.59
1:A:456:PRO:HA	1:A:459:MET:HE2	1.86	0.58
1:B:644:MET:HE3	1:B:854:GLY:HA2	1.83	0.58
1:B:454:LEU:HD11	1:B:459:MET:CG	2.29	0.58
1:B:559:GLU:HA	1:B:966:LYS:HE2	1.84	0.58
1:B:1119:LYS:HB2	1:B:1119:LYS:HZ3	1.66	0.58
1:A:887:PHE:CZ	1:A:909:MET:HE1	2.38	0.58
1:B:653:ARG:NH2	1:B:924:GLN:O	2.37	0.58
1:A:347:PHE:CE2	1:A:475:VAL:HG23	2.39	0.58
1:A:567:ARG:NH1	1:A:1007:LEU:O	2.37	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:B:314:MET:HE1	1:B:479:VAL:HA	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:554:VAL:HG22	1:B:684:ALA:HB3	1.86	0.57
1:B:1093:ILE:HD11	1:B:1145:TYR:CG	2.40	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:356:VAL:HG12	1:A:394:HIS:CG	2.39	0.57
1:A:1050:ARG:NH2	1:A:1065:THR:OG1	2.37	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:B:644:MET:CE	1:B:648:ILE:HD11	2.36	0.56
1:A:314:MET:HG2	1:A:347:PHE:HZ	1.70	0.56
1:A:569:ASP:OD1	1:A:569:ASP:N	2.39	0.56
1:A:809:ALA:O	1:A:813:ILE:HG13	2.06	0.56
1:B:731:GLN:O	1:B:735:ILE:HG13	2.05	0.56
1:B:1154:ILE:HG22	1:B:1159:THR:HG23	1.87	0.56
1:A:694:MET:HE3	1:A:698:ASN:HD21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:865:VAL:HA	1:B:868:VAL:HG12	1.88	0.55
1:B:1119:LYS:O	1:B:1123:LEU:HB2	2.07	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: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:868:VAL:HG22	1:A:887:PHE:CE1	2.41	0.54
1:A:1123:LEU:HD13	1:A:1135:LEU:HD12	1.90	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:B:953:MET:HE2	1:B:955:LEU:HD21	1.90	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:A:1116:ILE:HD12	1:A:1116:ILE:H	1.73	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:A:577:ASP:OD1	1:A:579:SER:OG	2.26	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
1:A:565:VAL:HG21	1:A:1006:PHE:CD1	2.44	0.52
1:A:569:ASP:C	1:A:570:LEU:HD12	2.33	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:B:298:LEU:O	1:B:1077:LEU:CD2	2.58	0.52
1:B:294:THR:HA	1:B:309:MET:HE2	1.91	0.52
1:B:485:TYR:HA	1:B:489:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:MET:HE3	1:B:648:ILE:HD11	1.92	0.52
1:B:644:MET:HE2	1:B:648:ILE:CD1	2.39	0.52
1:B:651:THR:CG2	1:B:941:THR:H	2.22	0.52
1:B:1100:ALA:HB1	1:B:1101:PRO:HD2	1.91	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:591:ALA:HA	1:B:912:TYR:HD2	1.76	0.51
1:B:1119:LYS:O	1:B:1123:LEU:HD12	2.10	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:982:LYS:HD2	2:C:11:DOC:OP2	2.10	0.51
1:B:992:LEU:HD22	1:B:1149:ARG:CZ	2.41	0.51
1:A:596:VAL:HG21	1:A:604:VAL:HG22	1.93	0.51
1:B:691:PRO:CG	1:B:742:TYR:CE1	2.92	0.51
1:B:1145:TYR:OH	1:B:1149:ARG:NH1	2.44	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: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:HG13	1:B:242:ILE:O	2.11	0.50
1:A:887:PHE:CD2	1:A:888:PRO:HD2	2.47	0.50
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:A:747:TYR:C	1:A:749:ARG:H	2.19	0.50
1:B:548:LEU:HD23	1:B:689:PHE:HB3	1.94	0.50
1:B:608:THR:OG1	1:B:609:ASN:N	2.45	0.50
1:A:961:GLU:HB2	1:A:1179:TRP:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:THR:HG23	1:B:447:LEU:HD12	1.93	0.50
1:A:1164:LEU:HG	1:A:1164:LEU:O	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:246:ASP:OD1	1:B:840:ARG:NH2	2.44	0.49
1:B:1116:ILE:HB	1:B:1117:PRO:CD	2.38	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:300:PHE:N	1:B:1081:MET:HE1	2.28	0.49
1:B:354:ASP:OD1	1:B:355:GLU:N	2.45	0.49
1:B:1151:GLY:O	1:B:1155:GLN:HG3	2.13	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:B:551:GLU:HG3	1:B:844:MET:HE1	1.95	0.48
1:A:380:ASP:HB2	1:A:421:ASP:OD2	2.14	0.48
1:B:300:PHE:H	1:B:1081:MET:HE1	1.78	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: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:OD1	1:B:897:ASN:N	2.47	0.47
1:B:910:LEU:O	1:B:914:VAL:HG23	2.13	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: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:868:VAL:HG21	1:A:887:PHE:HE1	1.78	0.47
1:A:875:ASP:OD1	1:A:876:THR:HG23	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:SER:O	1:B:390:ARG:NH2	2.47	0.47
1:B:552:THR:O	1:B:686:ARG:N	2.44	0.47
1:B:654:LEU:HD23	1:B:762:VAL:HG11	1.96	0.47
1:B:1145:TYR:CZ	1:B:1149:ARG:HD2	2.50	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:645:TYR:O	1:B:646:PRO:C	2.56	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:B:649:MET:HE3	1:B:846:MET:SD	2.55	0.46
1:A:968:ARG:HG3	1:A:983:GLY:HA3	1.96	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: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:B:1023:CYS:HB3	1:B:1154:ILE:CD1	2.45	0.46
1:B:86:LEU:HD23	1:B:115:SER:HA	1.98	0.46
1:B:298:LEU:O	1:B:1077:LEU:HD23	2.16	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:501:PRO:HD2	1:B:518:MET:HB3	1.98	0.45
1:B:1111:ILE:HD12	1:B:1126:TRP:CZ3	2.51	0.45
1:A:676:THR:OG1	1:A:677:CYS:N	2.48	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1073:LEU:HD13	1:A:1108:PRO:HB3	1.99	0.44
1:A:689:PHE:CE2	1:A:752:VAL:HB	2.52	0.44
1:A:1147:ARG:NH2	1:A:1173:ARG:O	2.50	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:907:CYS:SG	1:B:946:VAL:HG13	2.57	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:A:876:THR:OG1	2:P:11:DOC:H2"	2.17	0.44
1:A:51:GLY:O	1:A:128:SER:OG	2.21	0.44
1:A:78:TRP:CZ3	1:A:80:THR:HG22	2.53	0.44
1:A:261:VAL:HB	1:A:497:CYS:HB3	1.99	0.44
1:A:895:LEU:HD23	1:A:895:LEU:H	1.82	0.44
1:A:1083:LYS:HG2	1:A:1084:ASP:OD1	2.17	0.44
1:B:560:SER:HB2	1:B:966:LYS:HG2	2.00	0.44
1:B:644:MET:HE2	1:B:648:ILE:HD12	1.98	0.44
1:B:737:LYS:O	1:B:739:LEU:N	2.44	0.44
1:B:1176:HIS:CG	1:B:1180:LEU:HD23	2.52	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:B:835:MET:HE2	1:B:835:MET:HB3	1.78	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:652:ASN:HB2	1:B:654:LEU:HG	2.00	0.44
1:A:560:SER:HB2	1:A:966:LYS:HG3	2.00	0.43
1:A:1011:THR:O	1:A:1015:CYS:N	2.49	0.43
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:78:TRP:CE3	1:B:80:THR:HG22	2.54	0.43
1:B:496:LEU:HB3	1:B:507:THR:HG21	1.99	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:SG	1:B:677:CYS:O	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ILE:HD12	1:B:761:ILE:O	2.18	0.43
1:A:458:LEU:C	1:A:461:PRO:HD2	2.44	0.43
1:A:1094:SER:OG	1:A:1105:ARG:HB3	2.18	0.43
1:B:950:TYR:HB3	1:B:972:PHE:O	2.19	0.43
1:B:968:ARG:HA	1:B:982:LYS:O	2.19	0.43
1:B:314:MET:HE2	1:B:347:PHE:CZ	2.54	0.43
1:B:1116:ILE:CB	1:B:1117:PRO:HD3	2.46	0.43
1:A:905:TYR:CE2	1:A:909:MET:HE2	2.54	0.43
1:B:644:MET:HE2	1:B:648:ILE:HD11	2.01	0.43
1:B:865:VAL:HA	1:B:868:VAL:CG1	2.48	0.43
1:B:68:ASP:O	1:B:72:ILE:HD12	2.19	0.43
1:B:591:ALA:HA	1:B:912:TYR:CD2	2.53	0.43
3:D:6:DG:H2''	3:D:7:DA:H5'	2.00	0.43
1:A:50:MET:HA	1:A:50:MET:CE	2.45	0.42
1:A:295:LYS:HE3	1:A:295:LYS:HB3	1.95	0.42
1:B:835:MET:HE1	1:B:844:MET:HE2	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: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:404:PHE:CE2	1:A:414:SER:HB3	2.54	0.42
1:A:493:ILE:HD13	1:A:493:ILE:HA	1.80	0.42
1:A:992:LEU:HD23	1:A:995:ILE:HD12	2.01	0.42
1:A:1092:ILE:HG12	1:A:1109:VAL:HG12	2.01	0.42
1:B:121:PHE:HB3	1:B:129:PHE:CE2	2.54	0.42
1:B:1097:PRO:O	1:B:1100:ALA:HB3	2.20	0.42
1:A:1050:ARG:HB3	1:A:1050:ARG:HH11	1.85	0.42
1:A:177:MET:HE1	1:A:186:LYS:N	2.34	0.42
1:A:633:LEU:HD23	1:A:633:LEU:HA	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
1:B:845:GLU:O	1:B:849:ILE:HD12	2.19	0.42
1:B:1129:ASP:OD1	1:B:1131:SER:OG	2.28	0.42
1:A:680:LYS:HB3	1:A:680:LYS:HE3	1.93	0.42
1:B:121:PHE:CD2	1:B:129:PHE:CZ	3.08	0.42
1:B:1138:ARG:HH21	1:B:1138:ARG:CG	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:TYR:CD2	4:A:1301:DTP:H2'1	2.55	0.42
1:A:1133:GLU:O	1:A:1135:LEU:HD22	2.20	0.42
1:B:1052:MET:HE3	1:B:1052:MET:HB3	1.85	0.42
1:A:696:GLU:HA	1:A:699:MET:HE3	2.01	0.41
1:B:609:ASN:CG	1:B:894:THR:OG1	2.63	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: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: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:B:243:ARG:HE	1:B:243:ARG:HB3	1.76	0.41
1:B:799:ASP:C	1:B:801:SER:H	2.27	0.41
1:B:1002:ILE:HG12	1:B:1158:ILE:HD11	2.02	0.41
1:A:686:ARG:HD3	1:A:755:ILE:HG22	2.02	0.41
1:B:50:MET:HE1	1:B:370:ARG:HA	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:A:1101:PRO:HD2	1:A:1104:GLU:CD	2.45	0.41
2:P:5:DC:H2''	2:P:6:DG:C8	2.55	0.41
1:B:452:ILE:HD11	1:B:472:GLU:C	2.45	0.41
1:B:1150:LEU:HD23	1:B:1150:LEU:O	2.20	0.41
1:A:496:LEU:HB3	1:A:507:THR:HG21	2.02	0.41
1:A:887:PHE:HE2	1:A:909:MET:HE1	1.84	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:337:TYR:CE2	1:B:476:SER:HA	2.56	0.41
1:B:406:PRO:HD3	1:B:412:TYR:CE2	2.56	0.41
1:B:489:VAL:HG23	1:B:493:ILE:HG12	2.02	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: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:33:SER:O	1:A:36:GLN:N	2.52	0.41
1:B:402:ILE:O	1:B:416:TYR:OH	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ILE:N	1:A:355:GLU:OE1	2.44	0.40
1:A:347:PHE:HE2	1:A:475:VAL:HG23	1.85	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:319:GLY:HA3	1:A:347:PHE:CE1	2.57	0.40
1:A:1087:LEU:HD23	1:A:1089:CYS:SG	2.61	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:B:1040:GLU:O	1:B:1043:VAL:HG22	2.22	0.40
1:B:832:GLY:C	1:B:834:VAL:N	2.75	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%)	43 60
1	B	1082/1190 (91%)	1012 (94%)	66 (6%)	4 (0%)	30 45
All	All	2179/2380 (92%)	2047 (94%)	126 (6%)	6 (0%)	36 52

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%)	860 (99%)	7 (1%)	73	85
1	B	826/1066 (78%)	816 (99%)	10 (1%)	63	79
All	All	1693/2132 (79%)	1676 (99%)	17 (1%)	68	81

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	254	SER
1	A	454	LEU
1	A	588	LEU
1	A	628	ASN
1	A	629	ILE
1	A	630	ARG
1	A	1087	LEU
1	B	46	ILE
1	B	54	ARG
1	B	129	PHE
1	B	130	LYS
1	B	131	SER
1	B	243	ARG
1	B	291	ILE
1	B	1118	ILE
1	B	1119	LYS
1	B	1137	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	179	ASN
1	A	197	ASN
1	A	351	ASN
1	A	360	GLN
1	A	450	ASN
1	A	468	GLN
1	A	572	ASN
1	A	616	GLN
1	A	628	ASN
1	A	631	ASN
1	A	698	ASN
1	A	1062	GLN
1	A	1155	GLN
1	A	1176	HIS
1	B	185	GLN
1	B	198	GLN
1	B	324	ASN
1	B	915	HIS
1	B	916	GLN
1	B	973	ASN
1	B	999	GLN
1	B	1176	HIS

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	3,2	16,19,20	4.20	12 (75%)	20,26,29	1.22	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	DOC	P	11	3,2	16,19,20	4.17	12 (75%)	20,26,29	1.24	2 (10%)

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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	11	DOC	O4'-C4'	8.64	1.61	1.44
2	P	11	DOC	O4'-C4'	8.45	1.60	1.44
2	P	11	DOC	O4'-C1'	-6.94	1.26	1.42
2	C	11	DOC	O4'-C1'	-6.58	1.27	1.42
2	C	11	DOC	C2-N3	6.47	1.49	1.36
2	P	11	DOC	C2-N3	6.22	1.48	1.36
2	C	11	DOC	C6-C5	5.55	1.47	1.35
2	P	11	DOC	C6-C5	5.47	1.47	1.35
2	C	11	DOC	C4-N3	4.76	1.43	1.34
2	P	11	DOC	C4-N3	4.57	1.43	1.34
2	P	11	DOC	C3'-C4'	-3.98	1.32	1.52
2	C	11	DOC	C3'-C4'	-3.68	1.33	1.52
2	C	11	DOC	C4-N4	3.52	1.42	1.33
2	P	11	DOC	C2-N1	3.41	1.47	1.40
2	P	11	DOC	C4-N4	3.36	1.42	1.33
2	C	11	DOC	C2-N1	3.30	1.47	1.40
2	P	11	DOC	O2-C2	-3.00	1.18	1.23
2	C	11	DOC	O2-C2	-2.99	1.18	1.23
2	C	11	DOC	C6-N1	2.78	1.44	1.38
2	P	11	DOC	C6-N1	2.66	1.44	1.38
2	C	11	DOC	C2'-C1'	2.51	1.57	1.52
2	P	11	DOC	C2'-C1'	2.35	1.57	1.52
2	C	11	DOC	C5-C4	2.14	1.47	1.42
2	P	11	DOC	C5-C4	2.13	1.47	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	11	DOC	C3'-C2'-C1'	3.29	106.66	102.87
2	P	11	DOC	C4'-O4'-C1'	-3.03	106.95	109.81
2	C	11	DOC	C3'-C2'-C1'	2.75	106.03	102.87

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	C	11	DOC	5	0
2	P	11	DOC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	31,32,32	2.95	11 (35%)	46,50,50	2.26	15 (32%)
4	DTP	B	1301	5	31,32,32	2.95	11 (35%)	46,50,50	2.29	14 (30%)

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	-	2/22/34/34	0/3/3/3
4	DTP	B	1301	5	-	5/22/34/34	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	DTP	O4'-C4'	8.27	1.63	1.45
4	A	1301	DTP	C3'-C4'	-8.21	1.31	1.53
4	B	1301	DTP	O4'-C4'	8.19	1.63	1.45
4	B	1301	DTP	C3'-C4'	-8.16	1.31	1.53
4	B	1301	DTP	PA-O3A	4.44	1.64	1.59
4	A	1301	DTP	C6-N6	4.43	1.45	1.34
4	A	1301	DTP	O4'-C1'	-4.40	1.32	1.42
4	B	1301	DTP	C6-N6	4.30	1.45	1.34
4	B	1301	DTP	PB-O3A	4.27	1.64	1.59
4	B	1301	DTP	O4'-C1'	-4.23	1.32	1.42
4	A	1301	DTP	PB-O3B	4.12	1.64	1.59
4	A	1301	DTP	PB-O3A	4.07	1.63	1.59
4	B	1301	DTP	PB-O3B	3.56	1.63	1.59
4	A	1301	DTP	C5-N7	-3.06	1.33	1.39
4	A	1301	DTP	O3'-C3'	3.04	1.49	1.43
4	B	1301	DTP	C5-N7	-2.99	1.33	1.39
4	A	1301	DTP	C5-C4	-2.89	1.33	1.39
4	B	1301	DTP	C5-C4	-2.88	1.34	1.39
4	A	1301	DTP	PA-O3A	2.69	1.62	1.59
4	B	1301	DTP	O3'-C3'	2.62	1.48	1.43
4	A	1301	DTP	C8-N9	-2.43	1.33	1.37
4	B	1301	DTP	C8-N9	-2.35	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1301	DTP	N3-C2-N1	-5.77	119.85	128.58
4	B	1301	DTP	N6-C6-N1	-5.73	105.62	118.38
4	A	1301	DTP	N3-C2-N1	-5.44	120.35	128.58
4	A	1301	DTP	N6-C6-N1	-5.30	106.57	118.38
4	B	1301	DTP	C5-C4-N3	-4.86	120.02	126.72
4	A	1301	DTP	C1'-N9-C8	4.67	143.28	126.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1301	DTP	C4-N9-C1'	-4.63	107.92	126.50
4	A	1301	DTP	C5-C4-N3	-4.60	120.38	126.72
4	B	1301	DTP	C5-C6-N6	4.51	134.44	123.29
4	B	1301	DTP	C1'-N9-C8	4.40	142.34	126.95
4	B	1301	DTP	C4-N9-C1'	-4.37	108.99	126.50
4	A	1301	DTP	C5-C6-N6	4.19	133.65	123.29
4	B	1301	DTP	N9-C8-N7	-4.11	108.11	113.94
4	A	1301	DTP	N9-C8-N7	-3.99	108.27	113.94
4	B	1301	DTP	N3-C4-N9	3.68	133.42	127.17
4	A	1301	DTP	O3A-PA-O1A	-3.62	99.82	110.70
4	A	1301	DTP	N3-C4-N9	3.59	133.27	127.17
4	B	1301	DTP	C2-N3-C4	3.22	119.69	111.83
4	A	1301	DTP	C4-N9-C8	2.92	108.80	105.74
4	A	1301	DTP	C2-N3-C4	2.89	118.89	111.83
4	B	1301	DTP	C4-N9-C8	2.79	108.67	105.74
4	A	1301	DTP	C6-C5-C4	2.62	120.75	117.18
4	B	1301	DTP	C5-N7-C8	2.49	107.37	103.45
4	B	1301	DTP	C6-C5-C4	2.38	120.42	117.18
4	B	1301	DTP	O2B-PB-O3B	2.30	113.49	107.27
4	A	1301	DTP	C5-N7-C8	2.26	107.01	103.45
4	B	1301	DTP	O2A-PA-O3A	-2.07	101.68	107.27
4	A	1301	DTP	O2B-PB-O3A	2.01	112.72	107.27
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:

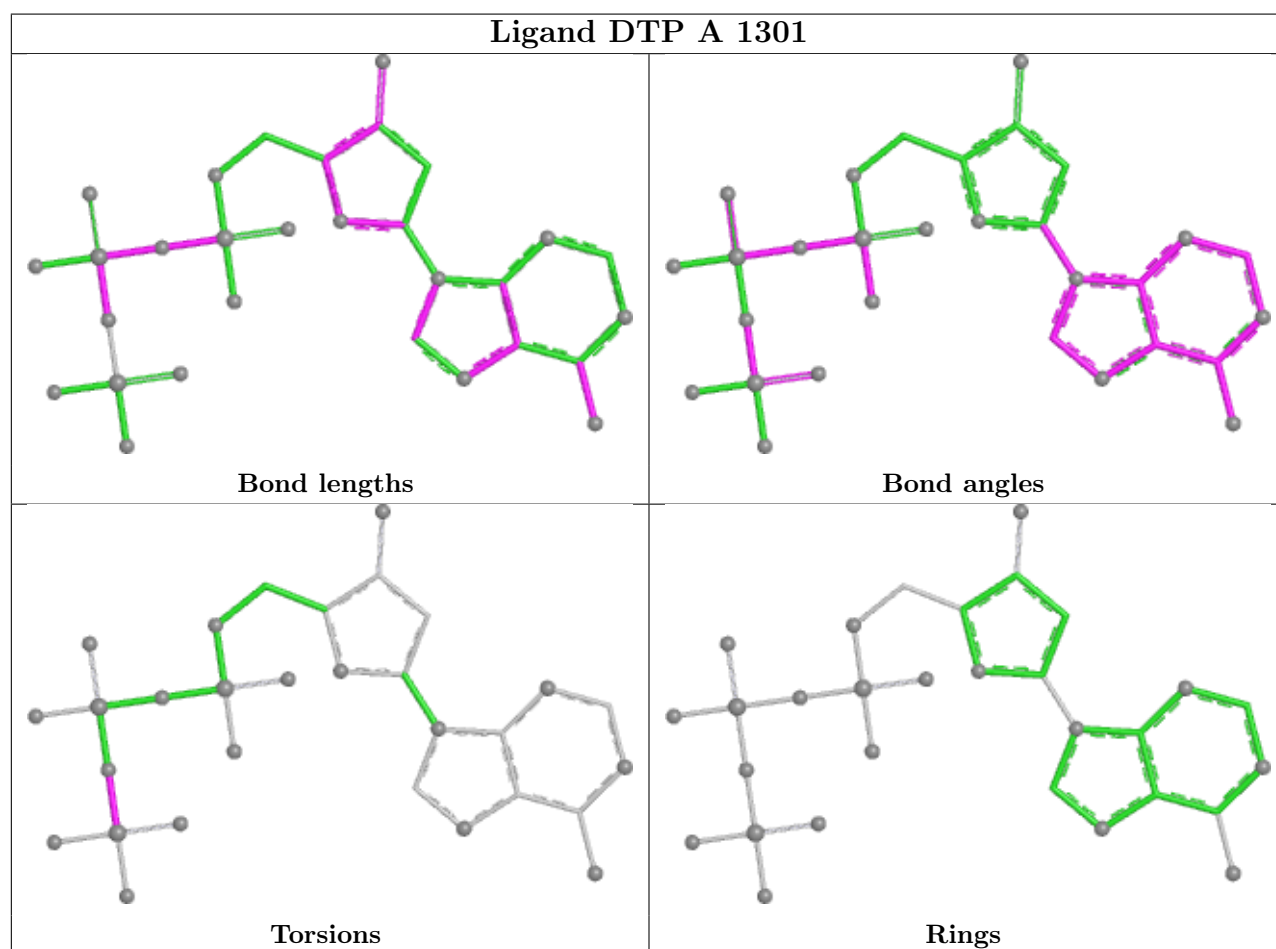
Mol	Chain	Res	Type	Atoms
4	A	1301	DTP	PB-O3B-PG-O3G
4	B	1301	DTP	C5'-O5'-PA-O1A
4	B	1301	DTP	C5'-O5'-PA-O2A
4	B	1301	DTP	C5'-O5'-PA-O3A
4	A	1301	DTP	PB-O3B-PG-O2G
4	B	1301	DTP	PB-O3B-PG-O3G
4	B	1301	DTP	C2'-C1'-N9-C8

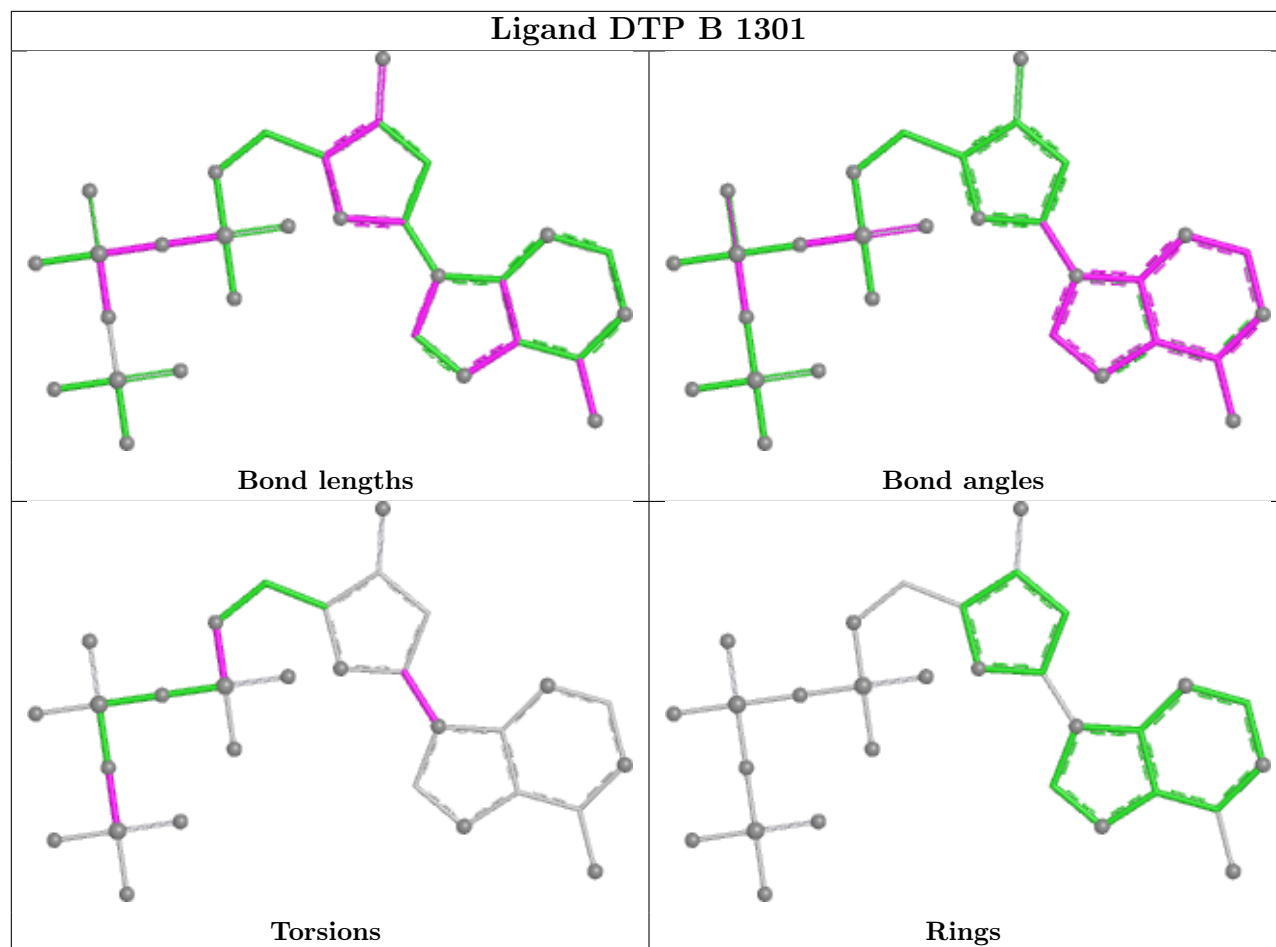
There are no ring outliers.

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%)	0.33	31 (2%)	55 48	50, 78, 101, 119	0
1	B	1094/1190 (91%)	0.44	39 (3%)	46 38	47, 81, 105, 123	0
2	C	10/11 (90%)	-0.13	0	100 100	54, 68, 81, 85	1 (10%)
2	P	10/11 (90%)	-0.15	0	100 100	52, 65, 76, 80	1 (10%)
3	D	15/16 (93%)	0.10	0	100 100	49, 67, 87, 99	0
3	T	15/16 (93%)	-0.09	0	100 100	48, 63, 88, 97	0
All	All	2251/2434 (92%)	0.38	70 (3%)	51 43	47, 79, 104, 123	2 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	750	VAL	4.3
1	B	1099	ASN	4.1
1	B	578	PRO	3.9
1	B	1096	LYS	3.9
1	B	617	ILE	3.8
1	B	1095	SER	3.6
1	B	596	VAL	3.4
1	B	64	PHE	3.3
1	B	1140	ILE	3.3
1	B	734	HIS	3.2
1	B	328	ILE	3.2
1	A	751	LYS	3.1
1	A	31	ALA	3.1
1	B	585	LEU	3.0
1	B	894	THR	3.0
1	B	1185	ALA	2.9
1	B	690	PHE	2.8
1	A	893	PHE	2.8
1	A	1128	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	661	ALA	2.7
1	A	697	TYR	2.7
1	A	895	LEU	2.7
1	A	990	GLY	2.7
1	A	347	PHE	2.7
1	A	991	GLU	2.6
1	B	29	ASN	2.6
1	B	901	LEU	2.5
1	B	802	ASP	2.5
1	B	619	GLN	2.5
1	A	1050	ARG	2.5
1	B	1070	ALA	2.5
1	B	628	ASN	2.4
1	A	53	GLU	2.4
1	B	589	PRO	2.4
1	B	604	VAL	2.4
1	A	901	LEU	2.4
1	B	722	THR	2.4
1	B	1100	ALA	2.4
1	B	1114	ALA	2.4
1	B	1056	LEU	2.3
1	B	726	LEU	2.3
1	A	632	GLU	2.3
1	A	693	LYS	2.3
1	A	1185	ALA	2.3
1	A	695	ASP	2.3
1	A	588	LEU	2.3
1	A	709	PHE	2.2
1	B	129	PHE	2.2
1	B	613	ILE	2.2
1	B	238	LEU	2.2
1	B	464	PHE	2.2
1	A	480	ALA	2.2
1	A	1184	ILE	2.2
1	A	676	THR	2.2
1	A	112	GLN	2.2
1	B	1115	ASP	2.2
1	B	592	LEU	2.1
1	A	748	HIS	2.1
1	A	700	ILE	2.1
1	A	1180	LEU	2.1
1	B	588	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	735	ILE	2.1
1	B	114	ILE	2.1
1	B	308	ILE	2.1
1	B	479	VAL	2.1
1	B	752	VAL	2.1
1	A	1164	LEU	2.0
1	A	678	ALA	2.0
1	B	1069	THR	2.0
1	A	742	TYR	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	P	11	18/19	0.95	0.10	43,51,63,64	0
2	DOC	C	11	18/19	0.96	0.09	44,52,64,67	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.

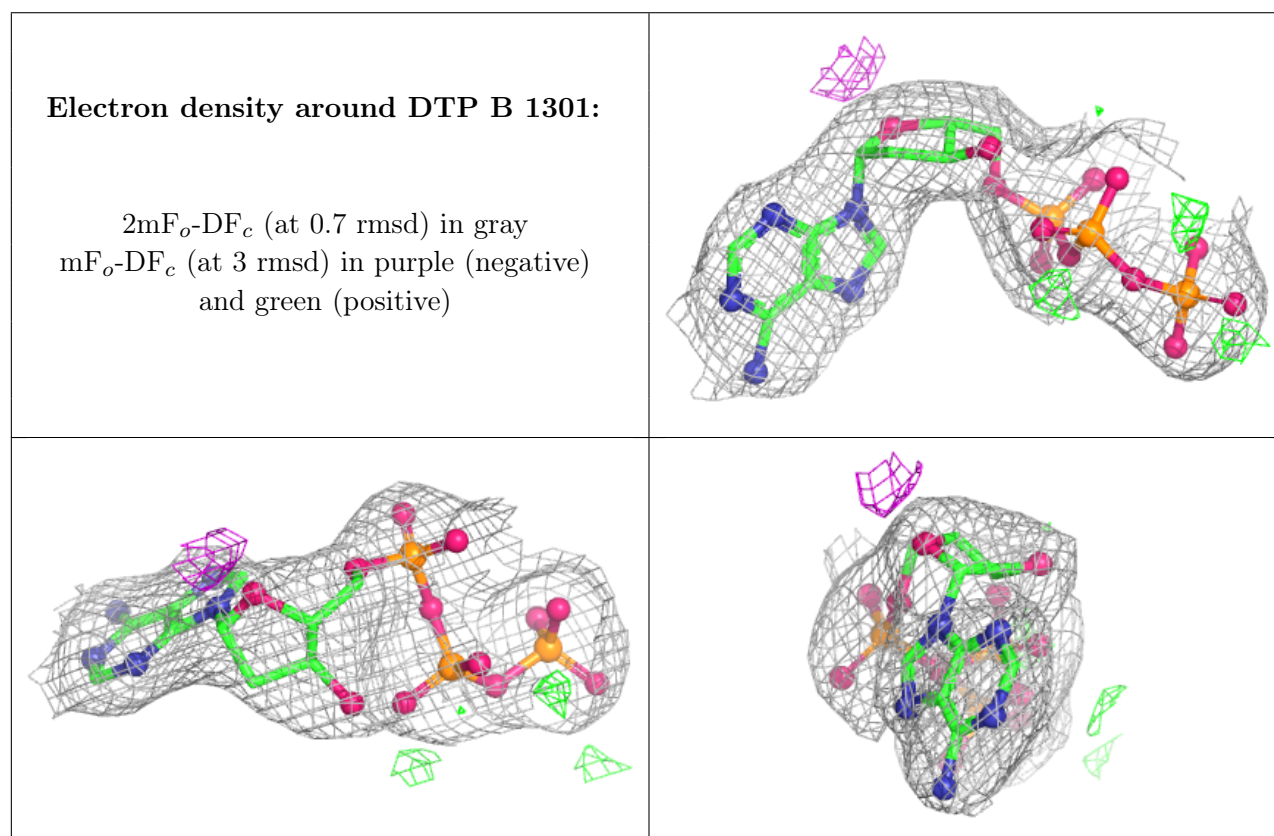
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	FE	A	1304	1/1	0.85	0.07	109,109,109,109	1
6	FE	B	1304	1/1	0.87	0.11	97,97,97,97	1
5	CA	A	1303	1/1	0.95	0.08	86,86,86,86	1
5	CA	B	1303	1/1	0.95	0.10	89,89,89,89	1
4	DTP	B	1301	30/30	0.96	0.08	44,52,61,67	0
4	DTP	A	1301	30/30	0.97	0.07	44,54,62,63	0
5	CA	B	1302	1/1	0.98	0.03	55,55,55,55	0

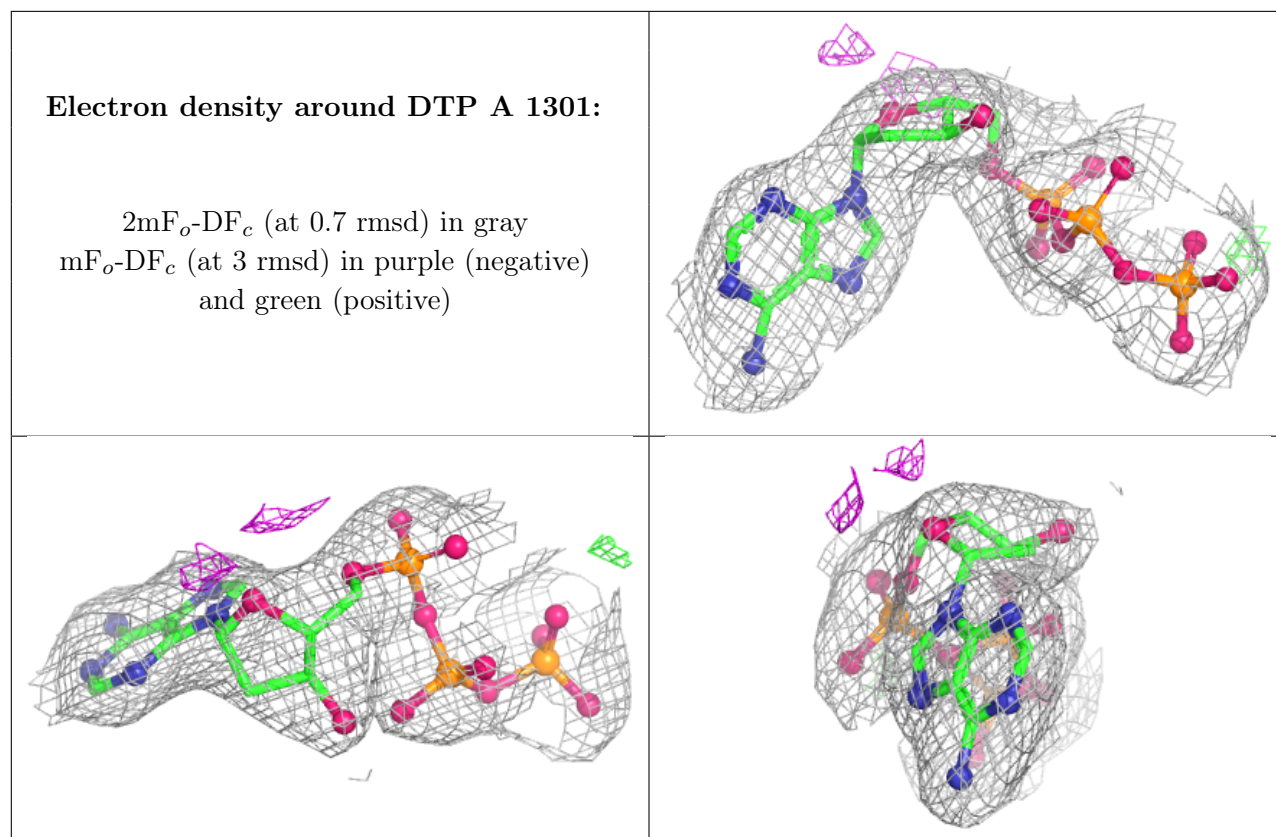
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CA	A	1302	1/1	0.99	0.04	63,63,63,63	0

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.





6.5 Other polymers [i](#)

There are no such residues in this entry.