



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:37 PM GMT

PDB ID : 1BPE
Title : CRYSTAL STRUCTURE OF RAT DNA POLYMERASE BETA; EVIDENCE FOR A COMMON POLYMERASE MECHANISM
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Deposited on : 1994-04-12
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

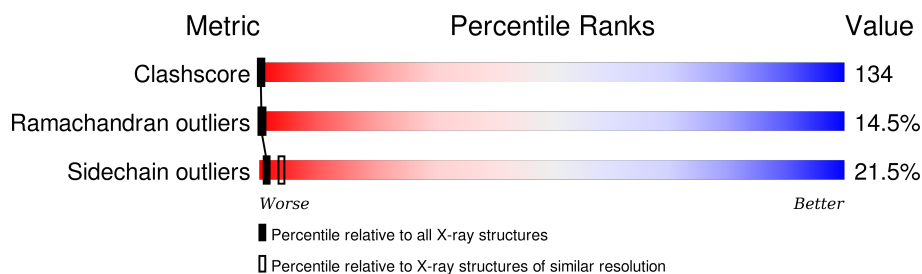
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	335	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DTP	A	338	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2158 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.

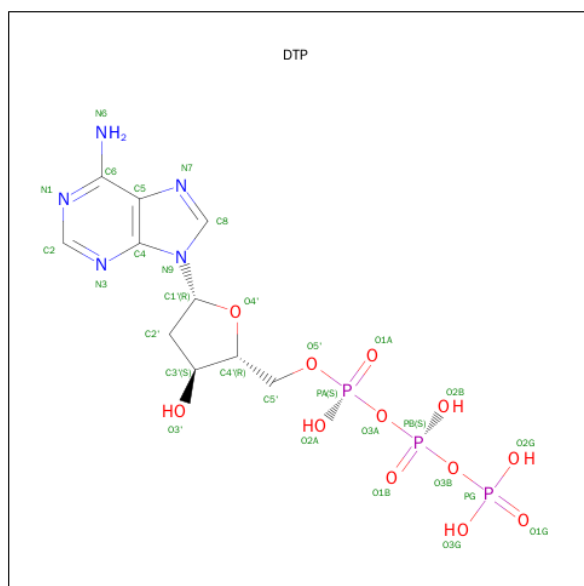
- Molecule 1 is a protein called DNA POLYMERASE BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2128	1335	377	408	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	ARG	GLN	CONFLICT	UNP P06766

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



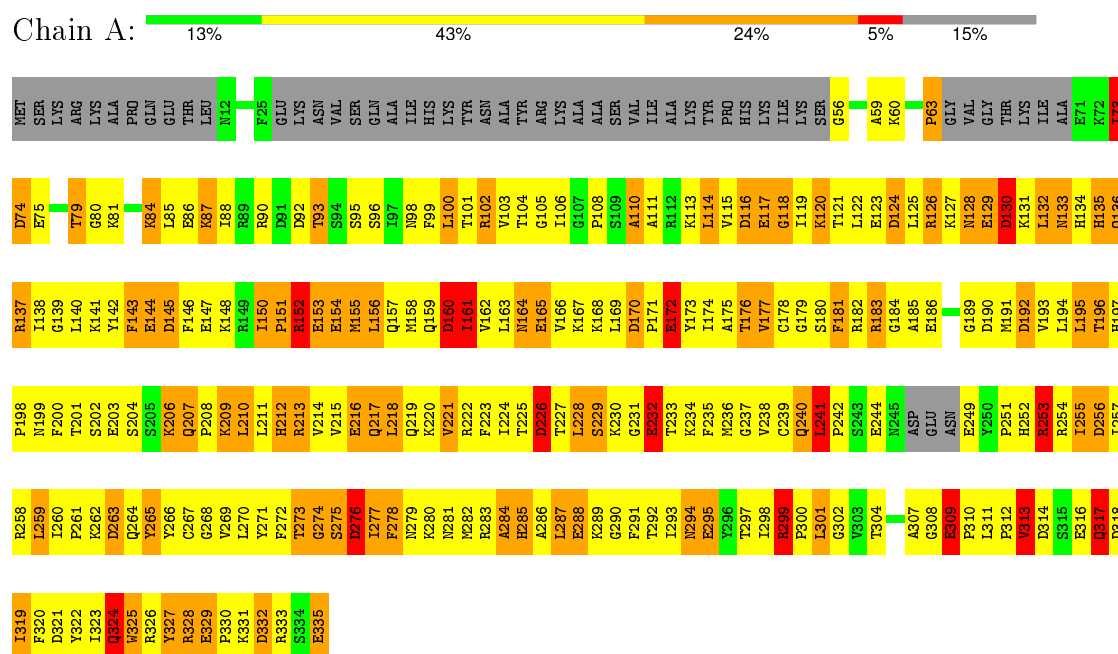
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			30	10	5	12	3		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

• Molecule 1: DNA POLYMERASE BETA



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.32Å 68.21Å 75.04Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2158	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.34	22/2165 (1.0%)	1.78	46/2926 (1.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	LYS	C-N	19.01	1.77	1.34
1	A	74	ASP	N-CA	8.00	1.62	1.46
1	A	288	GLU	CD-OE1	7.32	1.33	1.25
1	A	147	GLU	CD-OE1	6.83	1.33	1.25
1	A	153	GLU	CD-OE2	6.53	1.32	1.25
1	A	249	GLU	CD-OE1	6.51	1.32	1.25
1	A	203	GLU	CD-OE1	6.49	1.32	1.25
1	A	329	GLU	CD-OE1	6.44	1.32	1.25
1	A	165	GLU	CD-OE1	6.41	1.32	1.25
1	A	295	GLU	CD-OE1	6.39	1.32	1.25
1	A	144	GLU	CD-OE1	6.33	1.32	1.25
1	A	232	GLU	CD-OE1	6.27	1.32	1.25
1	A	172	GLU	CD-OE2	6.22	1.32	1.25
1	A	117	GLU	CD-OE1	6.17	1.32	1.25
1	A	186	GLU	CD-OE1	6.13	1.32	1.25
1	A	129	GLU	CD-OE2	5.99	1.32	1.25
1	A	335	GLU	CD-OE1	5.90	1.32	1.25
1	A	309	GLU	CD-OE1	5.49	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	216	GLU	CD-OE1	5.37	1.31	1.25
1	A	278	PHE	N-CA	-5.16	1.36	1.46
1	A	84	LYS	C-N	-5.12	1.22	1.34
1	A	154	GLU	CD-OE1	5.06	1.31	1.25

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	ILE	C-N-CD	-12.86	92.31	120.60
1	A	87	LYS	CA-C-N	-12.08	90.63	117.20
1	A	241	LEU	C-N-CD	-11.57	95.14	120.60
1	A	170	ASP	C-N-CD	-11.32	95.70	120.60
1	A	87	LYS	O-C-N	-10.15	106.46	122.70
1	A	256	ASP	CB-CG-OD1	-9.63	109.63	118.30
1	A	276	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	145	ASP	CB-CG-OD1	-7.92	111.17	118.30
1	A	318	ASP	CB-CG-OD1	-7.58	111.47	118.30
1	A	299	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	A	160	ASP	CB-CG-OD1	-7.25	111.77	118.30
1	A	275	SER	CB-CA-C	-7.25	96.33	110.10
1	A	130	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	74	ASP	N-CA-CB	-7.19	97.66	110.60
1	A	73	ILE	C-N-CA	-7.03	104.13	121.70
1	A	126	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	192	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	A	74	ASP	N-CA-C	6.71	129.11	111.00
1	A	130	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	192	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	63	PRO	N-CA-CB	6.37	110.94	103.30
1	A	318	ASP	CB-CG-OD2	6.32	123.99	118.30
1	A	222	ARG	CB-CA-C	6.31	123.03	110.40
1	A	124	ASP	CB-CG-OD1	-6.29	112.64	118.30
1	A	145	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	137	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	253	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	222	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	A	152	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	226	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	116	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	222	ARG	N-CA-CB	5.88	121.19	110.60
1	A	328	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	124	ASP	CB-CG-OD2	5.83	123.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	A	170	ASP	CB-CG-OD2	5.61	123.35	118.30
1	A	226	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	256	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	332	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	A	314	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	A	276	ASP	CB-CA-C	-5.54	99.32	110.40
1	A	314	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	196	THR	N-CA-CB	5.51	120.77	110.30
1	A	256	ASP	CB-CA-C	-5.38	99.64	110.40
1	A	263	ASP	CB-CG-OD1	-5.35	113.48	118.30
1	A	152	ARG	N-CA-CB	5.23	120.01	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	222	ARG	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	73	ILE	Peptide

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	2128	0	1946	536	2
2	A	30	0	12	15	0
All	All	2158	0	1958	551	2

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 134.

All (551) 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)
2:A:338:DTP:O1A	2:A:338:DTP:PA	1.10	1.49
1:A:87:LYS:C	1:A:88:ILE:N	1.77	1.38
2:A:338:DTP:C5'	2:A:338:DTP:PG	2.28	1.22
2:A:338:DTP:O2G	2:A:338:DTP:H5'2	1.37	1.17
2:A:338:DTP:H5'2	2:A:338:DTP:PG	1.84	1.17
1:A:241:LEU:HD23	1:A:242:PRO:HD2	1.27	1.13
1:A:317:GLN:NE2	1:A:317:GLN:H	1.52	1.08
1:A:309:GLU:HG3	1:A:310:PRO:HD2	1.32	1.06
1:A:122:LEU:HD13	1:A:126:ARG:HH12	1.22	1.04
2:A:338:DTP:H5'1	2:A:338:DTP:PG	1.92	1.04
1:A:100:LEU:HD23	1:A:115:VAL:HG22	1.40	1.03
1:A:259:LEU:HD12	1:A:260:ILE:H	1.22	1.00
1:A:104:THR:HB	1:A:139:GLY:HA3	1.42	1.00
1:A:289:LYS:HD2	1:A:323:ILE:HB	1.43	0.99
2:A:338:DTP:O1G	2:A:338:DTP:C5'	2.10	0.98
1:A:302:GLY:HA3	1:A:307:ALA:HB3	1.45	0.98
1:A:114:LEU:HA	1:A:117:GLU:HG2	1.46	0.98
1:A:218:LEU:HB3	1:A:224:ILE:HG13	1.45	0.97
1:A:56:GLY:HA2	1:A:59:ALA:HB3	1.42	0.97
1:A:319:ILE:HA	1:A:322:TYR:CD2	2.00	0.96
1:A:195:LEU:HD12	1:A:196:THR:H	1.31	0.93
1:A:104:THR:CB	1:A:139:GLY:HA3	1.99	0.92
1:A:106:ILE:HD12	1:A:111:ALA:HB2	1.47	0.92
1:A:99:PHE:HA	1:A:102:ARG:HE	1.32	0.92
1:A:319:ILE:HA	1:A:322:TYR:HD2	1.35	0.92
1:A:317:GLN:HE21	1:A:317:GLN:H	1.07	0.91
1:A:300:PRO:HD3	1:A:311:LEU:HD11	1.53	0.91
1:A:260:ILE:HG23	1:A:261:PRO:HD2	1.49	0.91
1:A:113:LYS:HG3	1:A:114:LEU:HD13	1.52	0.90
1:A:172:GLU:HG3	1:A:198:PRO:HG2	1.53	0.90
1:A:87:LYS:N	1:A:88:ILE:N	2.19	0.90
1:A:158:MET:HA	1:A:161:ILE:CD1	2.02	0.89
1:A:317:GLN:HE21	1:A:317:GLN:N	1.69	0.88
1:A:87:LYS:CA	1:A:88:ILE:N	2.36	0.88
1:A:286:ALA:HA	1:A:323:ILE:HG21	1.54	0.87
1:A:260:ILE:HG21	1:A:265:TYR:HA	1.55	0.87
1:A:289:LYS:CD	1:A:323:ILE:HB	2.05	0.87
1:A:261:PRO:HG2	1:A:264:GLN:HB2	1.56	0.86
1:A:309:GLU:HG3	1:A:310:PRO:CD	2.05	0.86
1:A:157:GLN:HB3	1:A:241:LEU:HD11	1.57	0.86
1:A:73:ILE:CB	1:A:75:GLU:H	1.88	0.85
1:A:56:GLY:CA	1:A:59:ALA:HB3	2.05	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ILE:HG12	1:A:253:ARG:CZ	2.07	0.85
1:A:100:LEU:CD2	1:A:115:VAL:HG22	2.06	0.84
1:A:270:LEU:HD22	1:A:319:ILE:HD11	1.59	0.84
1:A:99:PHE:HB2	1:A:102:ARG:HH21	1.42	0.84
1:A:259:LEU:HD12	1:A:260:ILE:N	1.92	0.83
1:A:330:PRO:HA	1:A:333:ARG:CD	2.07	0.83
1:A:143:PHE:HA	1:A:146:PHE:HB2	1.60	0.83
2:A:338:DTP:O2G	2:A:338:DTP:C5'	2.16	0.83
1:A:241:LEU:HD23	1:A:242:PRO:CD	2.10	0.81
2:A:338:DTP:H5'1	2:A:338:DTP:O3B	1.75	0.81
1:A:285:HIS:HA	1:A:288:GLU:HB2	1.63	0.81
1:A:294:ASN:ND2	1:A:299:ARG:NH1	2.28	0.81
1:A:302:GLY:CA	1:A:307:ALA:HB3	2.10	0.81
1:A:234:LYS:HG3	1:A:235:PHE:N	1.94	0.81
1:A:234:LYS:NZ	1:A:258:ARG:HH22	1.78	0.81
1:A:209:LYS:HA	1:A:212:HIS:HB2	1.64	0.80
1:A:209:LYS:CA	1:A:212:HIS:HB2	2.12	0.80
1:A:182:ARG:HH11	1:A:273:THR:HG21	1.46	0.80
1:A:173:TYR:CD1	1:A:195:LEU:HD11	2.17	0.79
1:A:207:GLN:HB3	1:A:210:LEU:HD12	1.63	0.79
1:A:150:ILE:HG12	1:A:253:ARG:NH1	1.97	0.79
1:A:139:GLY:O	1:A:143:PHE:HB2	1.82	0.79
1:A:113:LYS:HA	1:A:116:ASP:HB2	1.63	0.79
1:A:234:LYS:HZ2	1:A:258:ARG:NH2	1.80	0.79
1:A:228:LEU:HD23	1:A:237:GLY:HA2	1.65	0.79
1:A:265:TYR:O	1:A:269:VAL:HG23	1.82	0.79
1:A:202:SER:N	1:A:261:PRO:HB3	1.98	0.79
1:A:227:THR:HG23	1:A:235:PHE:HE1	1.46	0.78
1:A:319:ILE:HG12	1:A:320:PHE:N	1.97	0.78
1:A:211:LEU:HB2	1:A:259:LEU:HD23	1.65	0.78
1:A:270:LEU:HD12	1:A:333:ARG:HH12	1.48	0.78
1:A:114:LEU:HA	1:A:117:GLU:CG	2.14	0.78
1:A:155:MET:O	1:A:158:MET:HG2	1.83	0.78
1:A:157:GLN:HB3	1:A:241:LEU:CD1	2.14	0.78
1:A:161:ILE:HA	1:A:164:ASN:CG	2.04	0.77
1:A:122:LEU:HD13	1:A:126:ARG:NH1	2.00	0.77
1:A:204:SER:O	1:A:206:LYS:HG2	1.84	0.77
1:A:110:ALA:HA	1:A:113:LYS:CE	2.14	0.77
1:A:231:GLY:O	1:A:232:GLU:HG2	1.85	0.77
1:A:274:GLY:HA2	1:A:279:ASN:OD1	1.84	0.77
1:A:111:ALA:O	1:A:115:VAL:HG23	1.84	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:HIS:CG	1:A:198:PRO:HD2	2.20	0.77
1:A:221:VAL:CG2	1:A:223:PHE:H	1.98	0.76
1:A:234:LYS:NZ	1:A:258:ARG:NH2	2.33	0.76
1:A:241:LEU:CD2	1:A:242:PRO:HD2	2.12	0.76
1:A:330:PRO:HA	1:A:333:ARG:HD2	1.66	0.76
1:A:122:LEU:HD22	1:A:126:ARG:NH1	2.01	0.76
1:A:182:ARG:NH1	1:A:273:THR:HG21	2.01	0.75
1:A:201:THR:C	1:A:261:PRO:HB3	2.05	0.75
1:A:114:LEU:CA	1:A:117:GLU:HG2	2.16	0.75
1:A:131:LYS:O	1:A:132:LEU:HD13	1.86	0.75
1:A:287:LEU:HA	1:A:291:PHE:H	1.49	0.75
1:A:191:MET:HB3	1:A:255:ILE:HB	1.69	0.75
1:A:277:ILE:HD13	1:A:277:ILE:H	1.50	0.75
1:A:165:GLU:OE1	1:A:168:LYS:HE3	1.87	0.75
1:A:122:LEU:HB3	1:A:126:ARG:NH1	2.01	0.75
1:A:158:MET:HA	1:A:161:ILE:HD12	1.68	0.74
1:A:104:THR:CG2	1:A:139:GLY:HA3	2.17	0.74
1:A:253:ARG:HG2	1:A:253:ARG:HH11	1.52	0.74
1:A:286:ALA:CB	1:A:323:ILE:HG21	2.18	0.74
1:A:311:LEU:HD12	1:A:311:LEU:H	1.52	0.74
1:A:134:HIS:HA	1:A:137:ARG:NH1	2.03	0.73
1:A:197:HIS:CD2	1:A:198:PRO:HD2	2.22	0.73
1:A:195:LEU:HD12	1:A:196:THR:N	2.01	0.73
1:A:286:ALA:CA	1:A:323:ILE:HG21	2.18	0.73
1:A:106:ILE:HG22	1:A:136:GLN:NE2	2.02	0.73
1:A:183:ARG:HD3	1:A:333:ARG:HB2	1.68	0.73
1:A:110:ALA:HA	1:A:113:LYS:NZ	2.03	0.73
1:A:311:LEU:HB3	1:A:312:PRO:HD2	1.70	0.73
1:A:100:LEU:CD1	1:A:125:LEU:HD11	2.17	0.73
1:A:221:VAL:HG23	1:A:223:PHE:H	1.54	0.72
1:A:110:ALA:HA	1:A:113:LYS:HE3	1.70	0.72
1:A:261:PRO:HG2	1:A:264:GLN:CB	2.20	0.72
1:A:145:ASP:OD2	1:A:251:PRO:HB3	1.89	0.72
1:A:287:LEU:HD12	1:A:287:LEU:O	1.89	0.72
1:A:122:LEU:HB3	1:A:126:ARG:HH11	1.54	0.72
1:A:135:HIS:HB3	1:A:136:GLN:HG3	1.69	0.72
2:A:338:DTP:O2B	2:A:338:DTP:O1A	2.08	0.72
1:A:294:ASN:ND2	1:A:299:ARG:HH12	1.86	0.72
1:A:80:GLY:HA3	1:A:84:LYS:CB	2.20	0.72
1:A:158:MET:HG3	1:A:191:MET:CE	2.19	0.71
1:A:99:PHE:HD1	1:A:102:ARG:NE	1.87	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HG23	1:A:261:PRO:CD	2.21	0.71
1:A:215:VAL:O	1:A:219:GLN:HG3	1.91	0.71
1:A:150:ILE:HD11	1:A:253:ARG:CB	2.21	0.71
1:A:330:PRO:HA	1:A:333:ARG:HG3	1.73	0.71
1:A:110:ALA:O	1:A:114:LEU:HD22	1.90	0.71
1:A:131:LYS:C	1:A:132:LEU:HD22	2.12	0.70
1:A:119:ILE:O	1:A:120:LYS:HG3	1.89	0.70
1:A:122:LEU:HD22	1:A:126:ARG:CZ	2.21	0.70
1:A:270:LEU:HD22	1:A:319:ILE:CD1	2.21	0.70
1:A:113:LYS:O	1:A:117:GLU:N	2.25	0.70
1:A:294:ASN:N	1:A:294:ASN:HD22	1.88	0.69
1:A:132:LEU:HD22	1:A:132:LEU:N	2.07	0.69
1:A:228:LEU:CD2	1:A:237:GLY:HA2	2.22	0.69
1:A:326:ARG:O	1:A:328:ARG:N	2.25	0.69
1:A:330:PRO:HA	1:A:333:ARG:CG	2.23	0.69
1:A:169:LEU:HD11	1:A:217:GLN:HG2	1.75	0.69
1:A:284:ALA:O	1:A:288:GLU:N	2.26	0.69
1:A:105:GLY:HA3	1:A:136:GLN:HG2	1.75	0.69
1:A:134:HIS:O	1:A:138:ILE:HG12	1.93	0.69
1:A:142:TYR:O	1:A:144:GLU:N	2.26	0.68
1:A:209:LYS:C	1:A:212:HIS:HB2	2.14	0.68
1:A:281:ASN:O	1:A:284:ALA:HB3	1.94	0.68
1:A:300:PRO:O	1:A:308:GLY:HA2	1.94	0.68
1:A:158:MET:HG3	1:A:191:MET:HE1	1.74	0.68
1:A:117:GLU:C	1:A:119:ILE:H	1.96	0.68
1:A:106:ILE:HB	1:A:110:ALA:CB	2.25	0.67
1:A:172:GLU:HG3	1:A:198:PRO:CG	2.23	0.67
1:A:152:ARG:NH2	1:A:184:GLY:HA2	2.09	0.67
1:A:316:GLU:OE1	1:A:333:ARG:NH2	2.27	0.67
1:A:260:ILE:CG2	1:A:265:TYR:HA	2.24	0.67
1:A:85:LEU:C	1:A:87:LYS:H	1.97	0.67
1:A:227:THR:HG23	1:A:235:PHE:CE1	2.30	0.67
1:A:150:ILE:HG22	1:A:151:PRO:N	2.11	0.66
1:A:328:ARG:NH1	1:A:332:ASP:O	2.28	0.66
1:A:100:LEU:O	1:A:106:ILE:HD11	1.94	0.66
1:A:217:GLN:O	1:A:221:VAL:HG13	1.94	0.66
1:A:254:ARG:NH1	1:A:255:ILE:O	2.29	0.66
1:A:254:ARG:NH1	1:A:256:ASP:OD1	2.27	0.66
1:A:183:ARG:NH1	1:A:273:THR:O	2.27	0.66
1:A:100:LEU:HD11	1:A:125:LEU:HD11	1.75	0.66
1:A:297:THR:O	1:A:299:ARG:NH1	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:LEU:HD23	1:A:232:GLU:O	1.96	0.66
1:A:106:ILE:HB	1:A:110:ALA:HB3	1.76	0.66
1:A:162:VAL:HG12	1:A:163:LEU:N	2.11	0.66
1:A:217:GLN:O	1:A:220:LYS:N	2.29	0.65
1:A:277:ILE:HG12	1:A:278:PHE:N	2.10	0.65
1:A:287:LEU:HD11	1:A:301:LEU:HD22	1.78	0.65
1:A:209:LYS:O	1:A:213:ARG:N	2.29	0.65
1:A:311:LEU:HD12	1:A:311:LEU:N	2.11	0.65
1:A:229:SER:OG	1:A:230:LYS:N	2.28	0.65
1:A:183:ARG:CD	1:A:333:ARG:HB2	2.26	0.65
1:A:130:ASP:N	1:A:130:ASP:OD1	2.29	0.65
1:A:330:PRO:CA	1:A:333:ARG:HG3	2.27	0.65
1:A:253:ARG:HH11	1:A:253:ARG:CG	2.10	0.64
1:A:143:PHE:O	1:A:146:PHE:HB2	1.98	0.64
1:A:93:THR:O	1:A:96:SER:HB2	1.97	0.64
1:A:261:PRO:CG	1:A:264:GLN:HB2	2.28	0.64
1:A:110:ALA:C	1:A:114:LEU:HD22	2.16	0.64
1:A:152:ARG:NH2	1:A:181:PHE:O	2.29	0.64
1:A:276:ASP:O	1:A:279:ASN:N	2.29	0.64
1:A:166:VAL:O	1:A:169:LEU:N	2.30	0.64
1:A:143:PHE:CA	1:A:146:PHE:HB2	2.27	0.64
1:A:183:ARG:O	1:A:331:LYS:HA	1.97	0.64
1:A:276:ASP:O	1:A:280:LYS:N	2.31	0.64
1:A:286:ALA:HA	1:A:323:ILE:CG2	2.24	0.64
1:A:119:ILE:HA	1:A:124:ASP:OD2	1.98	0.64
1:A:73:ILE:CB	1:A:75:GLU:N	2.59	0.63
1:A:286:ALA:O	1:A:291:PHE:N	2.31	0.63
1:A:161:ILE:HA	1:A:164:ASN:OD1	1.99	0.63
1:A:298:ILE:HG12	1:A:311:LEU:HD13	1.80	0.63
1:A:106:ILE:CD1	1:A:111:ALA:HB2	2.24	0.63
1:A:236:MET:HA	1:A:256:ASP:HA	1.79	0.63
1:A:331:LYS:NZ	1:A:332:ASP:OD2	2.31	0.62
1:A:98:ASN:O	1:A:101:THR:HG22	1.99	0.62
2:A:338:DTP:O1G	2:A:338:DTP:C4'	2.47	0.62
2:A:338:DTP:O1G	2:A:338:DTP:H5'1	1.90	0.62
1:A:289:LYS:HZ2	1:A:323:ILE:HD12	1.63	0.62
1:A:173:TYR:O	1:A:174:ILE:HG13	1.98	0.62
1:A:123:GLU:HA	1:A:126:ARG:HB2	1.81	0.62
1:A:105:GLY:HA3	1:A:136:GLN:CG	2.30	0.62
1:A:204:SER:HG	1:A:206:LYS:HG3	1.64	0.62
1:A:261:PRO:HB2	1:A:263:ASP:OD1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:CG2	1:A:136:GLN:HA	2.30	0.62
1:A:138:ILE:C	1:A:140:LEU:H	2.03	0.62
1:A:150:ILE:HD11	1:A:253:ARG:CG	2.30	0.61
1:A:260:ILE:HG22	1:A:261:PRO:O	2.01	0.61
1:A:270:LEU:CD2	1:A:319:ILE:HD11	2.29	0.61
1:A:267:CYS:SG	1:A:297:THR:HA	2.40	0.61
1:A:122:LEU:CD1	1:A:126:ARG:HH12	2.07	0.61
1:A:113:LYS:O	1:A:117:GLU:HG2	2.00	0.61
1:A:238:VAL:HG12	1:A:252:HIS:HB3	1.82	0.61
1:A:151:PRO:HG2	1:A:154:GLU:CD	2.21	0.60
1:A:183:ARG:HD2	1:A:330:PRO:O	2.01	0.60
1:A:312:PRO:O	1:A:313:VAL:HG23	2.02	0.60
1:A:298:ILE:HG23	1:A:311:LEU:HD13	1.83	0.60
1:A:278:PHE:CZ	1:A:328:ARG:HD3	2.36	0.60
1:A:104:THR:HG22	1:A:136:GLN:HA	1.83	0.60
1:A:204:SER:HG	1:A:206:LYS:CG	2.14	0.60
1:A:234:LYS:HD2	1:A:236:MET:SD	2.42	0.60
1:A:270:LEU:HD12	1:A:333:ARG:NH1	2.17	0.60
1:A:227:THR:CG2	1:A:235:PHE:HE1	2.13	0.59
1:A:311:LEU:H	1:A:311:LEU:CD1	2.15	0.59
1:A:110:ALA:HA	1:A:113:LYS:HZ1	1.67	0.59
1:A:191:MET:HG3	1:A:192:ASP:H	1.68	0.59
1:A:182:ARG:HH11	1:A:273:THR:CG2	2.13	0.59
1:A:193:VAL:C	1:A:194:LEU:HD12	2.23	0.59
1:A:270:LEU:HD21	1:A:282:MET:CE	2.32	0.59
1:A:300:PRO:HD3	1:A:311:LEU:CD1	2.28	0.59
1:A:163:LEU:HA	1:A:166:VAL:HG13	1.84	0.59
1:A:275:SER:HG	1:A:277:ILE:HG12	1.66	0.59
1:A:155:MET:O	1:A:159:GLN:N	2.28	0.59
1:A:218:LEU:HB3	1:A:224:ILE:CG1	2.27	0.58
1:A:309:GLU:CG	1:A:310:PRO:HD2	2.21	0.58
1:A:113:LYS:HG3	1:A:114:LEU:CD1	2.31	0.58
1:A:289:LYS:NZ	1:A:323:ILE:O	2.36	0.58
1:A:299:ARG:HH11	1:A:299:ARG:HG3	1.67	0.58
1:A:92:ASP:O	1:A:95:SER:HB3	2.03	0.58
1:A:105:GLY:CA	1:A:136:GLN:HG2	2.33	0.58
1:A:134:HIS:ND1	1:A:137:ARG:NH2	2.51	0.58
1:A:106:ILE:N	1:A:136:GLN:HG2	2.19	0.58
1:A:236:MET:HE3	1:A:254:ARG:NH2	2.20	0.57
1:A:197:HIS:CE1	1:A:199:ASN:HB2	2.40	0.57
1:A:180:SER:O	1:A:183:ARG:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:O	1:A:221:VAL:HG22	2.04	0.57
1:A:284:ALA:O	1:A:287:LEU:N	2.38	0.57
1:A:218:LEU:HB2	1:A:224:ILE:HD12	1.87	0.56
1:A:278:PHE:HZ	1:A:328:ARG:HD3	1.69	0.56
1:A:156:LEU:HA	1:A:159:GLN:CB	2.35	0.56
1:A:285:HIS:O	1:A:289:LYS:HG3	2.06	0.56
1:A:99:PHE:CB	1:A:102:ARG:HH21	2.17	0.56
1:A:138:ILE:N	1:A:138:ILE:HD13	2.20	0.56
1:A:197:HIS:CE1	1:A:199:ASN:H	2.23	0.56
1:A:329:GLU:HB3	1:A:330:PRO:HD2	1.86	0.56
1:A:292:THR:HB	1:A:301:LEU:HD11	1.86	0.56
1:A:114:LEU:HD21	1:A:132:LEU:CD1	2.36	0.56
1:A:302:GLY:HA3	1:A:307:ALA:CB	2.29	0.56
1:A:60:LYS:HA	1:A:63:PRO:CB	2.36	0.56
1:A:143:PHE:C	1:A:146:PHE:HB2	2.26	0.56
2:A:338:DTP:O1G	2:A:338:DTP:H4'	2.06	0.56
1:A:317:GLN:HG3	1:A:327:TYR:CG	2.40	0.56
1:A:110:ALA:O	1:A:113:LYS:HG2	2.07	0.55
1:A:156:LEU:O	1:A:160:ASP:N	2.39	0.55
1:A:145:ASP:CG	1:A:251:PRO:HB3	2.26	0.55
1:A:218:LEU:HD22	1:A:218:LEU:H	1.71	0.55
1:A:260:ILE:CG2	1:A:261:PRO:HD2	2.32	0.55
1:A:191:MET:N	1:A:254:ARG:O	2.35	0.55
1:A:234:LYS:HZ3	1:A:258:ARG:HH22	1.54	0.55
1:A:216:GLU:O	1:A:219:GLN:HB2	2.06	0.55
1:A:234:LYS:HZ3	1:A:258:ARG:HH12	1.54	0.54
1:A:113:LYS:CA	1:A:116:ASP:HB2	2.36	0.54
2:A:338:DTP:O1A	2:A:338:DTP:PB	2.63	0.54
1:A:275:SER:OG	1:A:278:PHE:N	2.30	0.54
1:A:166:VAL:HG22	1:A:167:LYS:N	2.22	0.54
1:A:138:ILE:O	1:A:142:TYR:N	2.40	0.54
1:A:206:LYS:C	1:A:207:GLN:HG2	2.27	0.54
1:A:288:GLU:HA	1:A:288:GLU:OE1	2.08	0.54
1:A:172:GLU:HB3	1:A:197:HIS:CD2	2.42	0.54
1:A:207:GLN:C	1:A:209:LYS:HD2	2.28	0.54
1:A:278:PHE:HE2	1:A:328:ARG:NH1	2.06	0.53
1:A:253:ARG:NH1	1:A:253:ARG:HG2	2.22	0.53
1:A:172:GLU:HB3	1:A:197:HIS:NE2	2.22	0.53
1:A:197:HIS:ND1	1:A:199:ASN:N	2.51	0.53
1:A:172:GLU:CG	1:A:198:PRO:HG2	2.34	0.53
1:A:286:ALA:O	1:A:291:PHE:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:GLU:C	1:A:290:GLY:H	2.11	0.53
1:A:316:GLU:CD	1:A:333:ARG:HH22	2.12	0.53
1:A:158:MET:HG2	1:A:159:GLN:H	1.73	0.53
1:A:158:MET:HG2	1:A:159:GLN:N	2.23	0.53
1:A:285:HIS:ND1	1:A:325:TRP:CE2	2.77	0.53
1:A:135:HIS:O	1:A:138:ILE:HG12	2.09	0.53
1:A:268:GLY:HA2	1:A:295:GLU:O	2.09	0.53
1:A:204:SER:OG	1:A:207:GLN:NE2	2.34	0.53
1:A:232:GLU:HG3	1:A:233:THR:HG23	1.89	0.53
1:A:113:LYS:CG	1:A:114:LEU:HD13	2.31	0.53
1:A:150:ILE:CG2	1:A:151:PRO:HD2	2.39	0.53
1:A:99:PHE:HD1	1:A:102:ARG:CZ	2.22	0.53
1:A:90:ARG:O	1:A:93:THR:HG22	2.08	0.53
1:A:209:LYS:O	1:A:212:HIS:HB2	2.09	0.52
1:A:116:ASP:C	1:A:118:GLY:H	2.11	0.52
1:A:157:GLN:O	1:A:160:ASP:HB2	2.08	0.52
1:A:158:MET:HA	1:A:161:ILE:HD11	1.91	0.52
1:A:270:LEU:HD21	1:A:282:MET:HE2	1.90	0.52
1:A:254:ARG:HH22	1:A:256:ASP:CG	2.13	0.52
1:A:232:GLU:HG2	1:A:233:THR:H	1.75	0.52
1:A:287:LEU:HD11	1:A:301:LEU:CD2	2.39	0.52
1:A:117:GLU:O	1:A:119:ILE:N	2.42	0.52
1:A:261:PRO:HG3	1:A:264:GLN:OE1	2.10	0.52
1:A:113:LYS:HZ2	1:A:114:LEU:HD13	1.74	0.52
1:A:211:LEU:O	1:A:215:VAL:HG23	2.10	0.51
1:A:277:ILE:HD13	1:A:277:ILE:N	2.22	0.51
1:A:285:HIS:ND1	1:A:289:LYS:NZ	2.57	0.51
1:A:329:GLU:CB	1:A:330:PRO:HD2	2.40	0.51
1:A:142:TYR:HB2	1:A:146:PHE:CE2	2.45	0.51
1:A:204:SER:OG	1:A:206:LYS:HE3	2.10	0.51
1:A:207:GLN:O	1:A:210:LEU:HB2	2.10	0.51
1:A:317:GLN:HG3	1:A:327:TYR:CD2	2.45	0.51
1:A:142:TYR:HB3	1:A:146:PHE:CE1	2.46	0.51
1:A:234:LYS:HD2	1:A:236:MET:CG	2.41	0.51
1:A:260:ILE:HD12	1:A:261:PRO:HD2	1.92	0.51
1:A:142:TYR:CE1	1:A:252:HIS:CD2	2.98	0.51
1:A:221:VAL:HG22	1:A:223:PHE:H	1.74	0.51
1:A:110:ALA:CA	1:A:113:LYS:HE3	2.38	0.51
1:A:190:ASP:O	1:A:190:ASP:OD1	2.29	0.51
1:A:140:LEU:HG	1:A:141:LYS:N	2.23	0.51
1:A:142:TYR:CB	1:A:146:PHE:CZ	2.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:LEU:C	1:A:87:LYS:N	2.63	0.51
1:A:298:ILE:HD13	1:A:322:TYR:CD2	2.45	0.51
1:A:157:GLN:O	1:A:161:ILE:HG13	2.10	0.51
1:A:159:GLN:O	1:A:163:LEU:HG	2.11	0.51
1:A:122:LEU:O	1:A:126:ARG:HG3	2.11	0.51
1:A:114:LEU:HD21	1:A:132:LEU:HD11	1.91	0.51
1:A:87:LYS:C	1:A:88:ILE:CA	2.72	0.51
1:A:156:LEU:O	1:A:160:ASP:OD2	2.28	0.51
1:A:260:ILE:HG21	1:A:265:TYR:CA	2.34	0.51
1:A:286:ALA:HB2	1:A:323:ILE:HD13	1.93	0.51
1:A:106:ILE:HD12	1:A:111:ALA:CB	2.31	0.51
1:A:133:ASN:HD22	1:A:133:ASN:C	2.14	0.51
1:A:261:PRO:HG2	1:A:264:GLN:H	1.75	0.50
1:A:124:ASP:O	1:A:128:ASN:ND2	2.44	0.50
1:A:253:ARG:O	1:A:255:ILE:HG22	2.12	0.50
1:A:99:PHE:HA	1:A:102:ARG:NE	2.13	0.50
1:A:275:SER:OG	1:A:277:ILE:HG12	2.10	0.50
1:A:174:ILE:HD12	1:A:262:LYS:HE3	1.93	0.50
1:A:144:GLU:N	1:A:144:GLU:OE1	2.45	0.50
1:A:170:ASP:OD2	1:A:172:GLU:N	2.44	0.50
1:A:204:SER:OG	1:A:206:LYS:HG3	2.12	0.50
1:A:207:GLN:CB	1:A:210:LEU:HD12	2.39	0.50
1:A:279:ASN:O	1:A:283:ARG:HG2	2.11	0.50
1:A:116:ASP:O	1:A:118:GLY:N	2.41	0.49
1:A:142:TYR:HB2	1:A:146:PHE:CZ	2.47	0.49
1:A:100:LEU:HB3	1:A:111:ALA:HB1	1.94	0.49
1:A:191:MET:HG3	1:A:192:ASP:N	2.27	0.49
1:A:114:LEU:C	1:A:117:GLU:H	2.16	0.49
1:A:99:PHE:O	1:A:102:ARG:HB2	2.11	0.49
1:A:122:LEU:HD21	1:A:144:GLU:OE2	2.12	0.49
1:A:173:TYR:OH	1:A:210:LEU:O	2.29	0.49
1:A:174:ILE:HD12	1:A:262:LYS:NZ	2.27	0.49
1:A:323:ILE:O	1:A:324:GLN:O	2.31	0.49
1:A:138:ILE:HG22	1:A:142:TYR:HD2	1.77	0.49
1:A:141:LYS:NZ	1:A:142:TYR:CE1	2.80	0.49
1:A:168:LYS:NZ	1:A:168:LYS:HB3	2.28	0.49
1:A:143:PHE:HA	1:A:146:PHE:CB	2.39	0.49
1:A:193:VAL:O	1:A:194:LEU:HD12	2.13	0.49
1:A:221:VAL:HG23	1:A:223:PHE:N	2.24	0.48
1:A:169:LEU:HD21	1:A:217:GLN:OE1	2.13	0.48
1:A:285:HIS:ND1	1:A:325:TRP:CZ2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:THR:OG1	1:A:298:ILE:N	2.45	0.48
1:A:154:GLU:O	1:A:157:GLN:HB2	2.13	0.48
1:A:294:ASN:ND2	1:A:297:THR:H	2.11	0.48
1:A:298:ILE:CD1	1:A:322:TYR:CD2	2.96	0.48
1:A:152:ARG:NH2	1:A:184:GLY:CA	2.77	0.48
1:A:217:GLN:HA	1:A:217:GLN:HE21	1.78	0.48
1:A:217:GLN:O	1:A:219:GLN:N	2.46	0.48
1:A:98:ASN:O	1:A:102:ARG:HG3	2.14	0.48
1:A:156:LEU:CD1	1:A:181:PHE:HE2	2.27	0.48
1:A:100:LEU:HG	1:A:125:LEU:HD11	1.95	0.48
1:A:177:VAL:O	1:A:177:VAL:HG13	2.14	0.48
1:A:202:SER:HB3	1:A:264:GLN:HG3	1.95	0.48
1:A:114:LEU:CD2	1:A:132:LEU:HD11	2.43	0.48
1:A:100:LEU:CG	1:A:125:LEU:HD11	2.43	0.48
1:A:209:LYS:HA	1:A:212:HIS:CB	2.41	0.47
1:A:202:SER:OG	1:A:263:ASP:OD2	2.29	0.47
1:A:95:SER:O	1:A:99:PHE:HB3	2.14	0.47
1:A:279:ASN:O	1:A:283:ARG:HD3	2.14	0.47
1:A:293:ILE:HA	1:A:297:THR:O	2.14	0.47
1:A:317:GLN:NE2	1:A:317:GLN:N	2.33	0.47
1:A:197:HIS:HE1	1:A:199:ASN:CG	2.17	0.47
1:A:285:HIS:ND1	1:A:289:LYS:CE	2.77	0.47
1:A:285:HIS:CE1	1:A:325:TRP:HE1	2.33	0.47
1:A:99:PHE:CA	1:A:102:ARG:HE	2.17	0.47
1:A:133:ASN:HD21	1:A:135:HIS:HB3	1.78	0.47
1:A:265:TYR:HD2	1:A:266:TYR:CE1	2.32	0.47
1:A:275:SER:HG	1:A:278:PHE:H	1.58	0.47
2:A:338:DTP:O5'	2:A:338:DTP:H8	2.15	0.47
1:A:196:THR:HA	1:A:259:LEU:HD11	1.97	0.47
1:A:165:GLU:O	1:A:169:LEU:HG	2.14	0.47
1:A:144:GLU:O	1:A:148:LYS:HE3	2.15	0.47
1:A:197:HIS:CE1	1:A:199:ASN:CB	2.98	0.47
1:A:229:SER:O	1:A:230:LYS:HB2	2.15	0.47
1:A:285:HIS:CG	1:A:289:LYS:HE3	2.50	0.47
1:A:311:LEU:HB3	1:A:312:PRO:CD	2.44	0.47
1:A:101:THR:O	1:A:103:VAL:O	2.32	0.47
1:A:232:GLU:CG	1:A:233:THR:N	2.77	0.46
1:A:104:THR:O	1:A:136:GLN:HG2	2.15	0.46
1:A:207:GLN:HB3	1:A:210:LEU:CD1	2.39	0.46
1:A:236:MET:CE	1:A:254:ARG:NH2	2.78	0.46
1:A:328:ARG:NH2	1:A:335:GLU:OXT	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:PHE:N	1:A:146:PHE:CD1	2.79	0.46
1:A:200:PHE:CD1	1:A:201:THR:N	2.83	0.46
1:A:276:ASP:HB2	1:A:277:ILE:HD13	1.98	0.46
1:A:115:VAL:O	1:A:119:ILE:O	2.33	0.46
1:A:207:GLN:N	1:A:208:PRO:CD	2.79	0.46
1:A:157:GLN:HB3	1:A:241:LEU:HD13	1.96	0.46
1:A:127:LYS:O	1:A:129:GLU:HG3	2.16	0.46
1:A:191:MET:CG	1:A:192:ASP:N	2.79	0.46
1:A:284:ALA:O	1:A:287:LEU:HB3	2.15	0.46
1:A:316:GLU:O	1:A:319:ILE:HG23	2.15	0.46
1:A:317:GLN:CG	1:A:327:TYR:CD2	2.99	0.46
1:A:179:GLY:HA2	1:A:272:PHE:O	2.15	0.46
1:A:174:ILE:HD12	1:A:262:LYS:CE	2.47	0.45
1:A:174:ILE:CD1	1:A:262:LYS:NZ	2.79	0.45
1:A:150:ILE:CG2	1:A:151:PRO:N	2.78	0.45
1:A:308:GLY:O	1:A:309:GLU:HB2	2.17	0.45
1:A:298:ILE:O	1:A:298:ILE:HG23	2.16	0.45
1:A:104:THR:HB	1:A:139:GLY:CA	2.29	0.45
1:A:99:PHE:CD1	1:A:102:ARG:CZ	3.00	0.45
1:A:266:TYR:HB2	1:A:313:VAL:CG1	2.46	0.45
1:A:99:PHE:CD1	1:A:102:ARG:NH2	2.85	0.45
1:A:190:ASP:HA	1:A:254:ARG:O	2.17	0.45
1:A:289:LYS:HD3	1:A:323:ILE:O	2.16	0.45
1:A:151:PRO:HG2	1:A:154:GLU:OE2	2.17	0.45
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.65	0.45
1:A:156:LEU:HD13	1:A:181:PHE:CE2	2.52	0.45
1:A:277:ILE:O	1:A:281:ASN:OD1	2.34	0.45
1:A:215:VAL:HG13	1:A:235:PHE:CE2	2.52	0.44
1:A:151:PRO:HG2	1:A:154:GLU:OE1	2.17	0.44
1:A:156:LEU:HD13	1:A:156:LEU:HA	1.63	0.44
1:A:234:LYS:HZ3	1:A:258:ARG:NH1	2.14	0.44
1:A:275:SER:O	1:A:279:ASN:OD1	2.35	0.44
1:A:311:LEU:CD1	1:A:311:LEU:N	2.77	0.44
1:A:234:LYS:NZ	1:A:258:ARG:CZ	2.81	0.44
1:A:136:GLN:H	1:A:136:GLN:HG3	1.48	0.44
1:A:271:TYR:CD2	1:A:295:GLU:HA	2.53	0.44
1:A:154:GLU:HA	1:A:157:GLN:HB2	1.99	0.44
1:A:113:LYS:NZ	1:A:114:LEU:HD13	2.32	0.44
1:A:271:TYR:CE2	1:A:295:GLU:HB3	2.52	0.44
1:A:116:ASP:C	1:A:118:GLY:N	2.71	0.44
1:A:106:ILE:HB	1:A:110:ALA:HB1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HA	1:A:114:LEU:HD12	1.69	0.44
1:A:211:LEU:HB2	1:A:259:LEU:CD2	2.44	0.44
1:A:329:GLU:O	1:A:333:ARG:HG3	2.18	0.44
1:A:114:LEU:CD1	1:A:114:LEU:N	2.80	0.44
1:A:236:MET:HA	1:A:256:ASP:OD1	2.17	0.43
1:A:151:PRO:C	1:A:153:GLU:H	2.21	0.43
1:A:202:SER:HB2	1:A:264:GLN:NE2	2.33	0.43
1:A:150:ILE:HD11	1:A:253:ARG:HB2	1.96	0.43
1:A:158:MET:HA	1:A:161:ILE:CG1	2.47	0.43
1:A:150:ILE:HG23	1:A:151:PRO:HD2	1.99	0.43
1:A:191:MET:O	1:A:192:ASP:HB2	2.18	0.43
1:A:331:LYS:CG	1:A:332:ASP:N	2.81	0.43
1:A:113:LYS:NZ	1:A:114:LEU:CD1	2.81	0.43
1:A:177:VAL:H	1:A:177:VAL:HG12	1.53	0.43
1:A:158:MET:HB2	1:A:223:PHE:CZ	2.54	0.43
1:A:196:THR:HA	1:A:259:LEU:CD1	2.48	0.43
1:A:285:HIS:CE1	1:A:325:TRP:NE1	2.86	0.43
1:A:172:GLU:O	1:A:198:PRO:HD3	2.18	0.43
1:A:236:MET:HE3	1:A:256:ASP:OD1	2.19	0.43
1:A:270:LEU:HD21	1:A:282:MET:HE1	2.00	0.43
1:A:311:LEU:CB	1:A:312:PRO:HD2	2.42	0.43
2:A:338:DTP:O1G	2:A:338:DTP:H5'2	1.89	0.43
1:A:165:GLU:HA	1:A:165:GLU:OE1	2.15	0.43
1:A:270:LEU:CD1	1:A:333:ARG:NH1	2.81	0.43
1:A:98:ASN:HA	1:A:101:THR:HG22	2.00	0.43
1:A:176:THR:N	1:A:194:LEU:O	2.51	0.43
1:A:103:VAL:CG1	1:A:104:THR:N	2.82	0.43
1:A:221:VAL:CG2	1:A:223:PHE:HB2	2.49	0.43
1:A:285:HIS:CA	1:A:288:GLU:HB2	2.41	0.43
1:A:110:ALA:O	1:A:113:LYS:NZ	2.47	0.43
1:A:261:PRO:C	1:A:263:ASP:H	2.21	0.42
1:A:260:ILE:CG2	1:A:265:TYR:CA	2.94	0.42
1:A:270:LEU:HD12	1:A:270:LEU:HA	1.64	0.42
1:A:100:LEU:HB3	1:A:111:ALA:CB	2.49	0.42
1:A:160:ASP:O	1:A:164:ASN:HB3	2.19	0.42
1:A:259:LEU:O	1:A:260:ILE:HD13	2.19	0.42
1:A:133:ASN:ND2	1:A:135:HIS:HB3	2.33	0.42
1:A:166:VAL:CG2	1:A:167:LYS:N	2.82	0.42
1:A:218:LEU:HD13	1:A:218:LEU:HA	1.87	0.42
1:A:218:LEU:HD22	1:A:218:LEU:N	2.34	0.42
1:A:236:MET:HE3	1:A:236:MET:HB3	1.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:VAL:HG13	1:A:120:LYS:HA	2.00	0.42
1:A:224:ILE:HD13	1:A:235:PHE:HE2	1.84	0.42
1:A:241:LEU:HA	1:A:242:PRO:HD2	1.76	0.42
1:A:278:PHE:C	1:A:280:LYS:H	2.22	0.42
1:A:221:VAL:HG13	1:A:221:VAL:H	1.14	0.42
1:A:99:PHE:CD1	1:A:102:ARG:NE	2.77	0.42
1:A:319:ILE:O	1:A:322:TYR:HB2	2.18	0.42
1:A:104:THR:HG22	1:A:139:GLY:HA3	1.96	0.42
1:A:150:ILE:HD11	1:A:253:ARG:HG2	1.99	0.42
1:A:163:LEU:CA	1:A:166:VAL:HG13	2.50	0.42
1:A:268:GLY:O	1:A:271:TYR:HB3	2.20	0.42
1:A:221:VAL:CG2	1:A:223:PHE:CB	2.97	0.41
1:A:261:PRO:C	1:A:263:ASP:N	2.72	0.41
1:A:100:LEU:HD23	1:A:115:VAL:CG2	2.30	0.41
1:A:96:SER:OG	1:A:120:LYS:HG2	2.20	0.41
1:A:240:GLN:HG2	1:A:241:LEU:O	2.21	0.41
1:A:287:LEU:CD1	1:A:301:LEU:HD22	2.46	0.41
1:A:115:VAL:HA	1:A:119:ILE:O	2.20	0.41
1:A:177:VAL:CG2	1:A:178:CYS:N	2.81	0.41
1:A:152:ARG:HA	1:A:155:MET:HB2	2.01	0.41
1:A:164:ASN:O	1:A:168:LYS:HG3	2.20	0.41
1:A:173:TYR:CD1	1:A:195:LEU:CD1	2.99	0.41
1:A:260:ILE:CG2	1:A:265:TYR:N	2.83	0.41
1:A:104:THR:OG1	1:A:105:GLY:N	2.52	0.41
1:A:111:ALA:HA	1:A:114:LEU:HB2	2.02	0.41
1:A:218:LEU:O	1:A:223:PHE:HB3	2.20	0.41
1:A:158:MET:CG	1:A:159:GLN:N	2.83	0.41
1:A:156:LEU:HD13	1:A:181:PHE:HE2	1.84	0.41
1:A:289:LYS:H	1:A:289:LYS:HG3	1.51	0.41
1:A:102:ARG:HB3	1:A:143:PHE:CE1	2.54	0.41
1:A:294:ASN:HD21	1:A:299:ARG:NH1	2.13	0.41
1:A:135:HIS:HB3	1:A:136:GLN:H	1.19	0.41
1:A:138:ILE:O	1:A:141:LYS:N	2.54	0.41
1:A:85:LEU:O	1:A:87:LYS:N	2.53	0.41
1:A:277:ILE:CD1	1:A:277:ILE:H	2.27	0.41
1:A:175:ALA:HA	1:A:194:LEU:O	2.21	0.41
1:A:157:GLN:HA	1:A:160:ASP:OD2	2.21	0.41
1:A:181:PHE:C	1:A:181:PHE:CD1	2.94	0.41
1:A:166:VAL:O	1:A:169:LEU:HB2	2.21	0.41
1:A:292:THR:HG22	1:A:301:LEU:HD12	2.02	0.41
1:A:103:VAL:HG12	1:A:104:THR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:LEU:HD13	1:A:114:LEU:N	2.35	0.41
1:A:150:ILE:HD13	1:A:253:ARG:HD3	2.03	0.41
1:A:292:THR:CB	1:A:301:LEU:HD11	2.51	0.41
1:A:291:PHE:HD2	1:A:323:ILE:HG22	1.86	0.41
1:A:330:PRO:O	1:A:333:ARG:HG3	2.21	0.41
1:A:113:LYS:CG	1:A:114:LEU:N	2.83	0.41
1:A:133:ASN:ND2	1:A:135:HIS:CB	2.84	0.41
1:A:163:LEU:HA	1:A:166:VAL:CG1	2.51	0.40
1:A:223:PHE:O	1:A:225:THR:N	2.54	0.40
1:A:234:LYS:HZ3	1:A:258:ARG:NH2	2.14	0.40
1:A:261:PRO:HB2	1:A:263:ASP:H	1.86	0.40
1:A:235:PHE:O	1:A:257:ILE:N	2.55	0.40
1:A:156:LEU:CD1	1:A:181:PHE:CE2	3.04	0.40
1:A:218:LEU:CB	1:A:224:ILE:CD1	2.99	0.40
1:A:239:CYS:HB2	1:A:240:GLN:H	1.73	0.40
1:A:122:LEU:CD2	1:A:126:ARG:NH1	2.79	0.40
1:A:92:ASP:O	1:A:95:SER:N	2.45	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:N	1:A:335:GLU:OE2[2_656]	2.06	0.14
1:A:226:ASP:CA	1:A:335:GLU:OE2[2_656]	2.11	0.09

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	276/335 (82%)	183 (66%)	53 (19%)	40 (14%)	0 0

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASP
1	A	79	THR
1	A	81	LYS
1	A	86	GLU
1	A	128	ASN
1	A	135	HIS
1	A	143	PHE
1	A	185	ALA
1	A	244	GLU
1	A	304	THR
1	A	309	GLU
1	A	324	GLN
1	A	73	ILE
1	A	110	ALA
1	A	118	GLY
1	A	120	LYS
1	A	130	ASP
1	A	136	GLN
1	A	218	LEU
1	A	240	GLN
1	A	274	GLY
1	A	301	LEU
1	A	327	TYR
1	A	151	PRO
1	A	160	ASP
1	A	189	GLY
1	A	232	GLU
1	A	284	ALA
1	A	102	ARG
1	A	152	ARG
1	A	276	ASP
1	A	317	GLN
1	A	171	PRO
1	A	161	ILE
1	A	183	ARG
1	A	207	GLN
1	A	228	LEU
1	A	265	TYR
1	A	108	PRO
1	A	313	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	205/296 (69%)	161 (78%)	44 (22%)	1 4

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	THR
1	A	93	THR
1	A	100	LEU
1	A	114	LEU
1	A	121	THR
1	A	132	LEU
1	A	133	ASN
1	A	152	ARG
1	A	155	MET
1	A	156	LEU
1	A	161	ILE
1	A	164	ASN
1	A	172	GLU
1	A	176	THR
1	A	177	VAL
1	A	181	PHE
1	A	195	LEU
1	A	206	LYS
1	A	209	LYS
1	A	210	LEU
1	A	212	HIS
1	A	213	ARG
1	A	214	VAL
1	A	217	GLN
1	A	221	VAL
1	A	226	ASP
1	A	229	SER
1	A	241	LEU
1	A	253	ARG
1	A	255	ILE

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Mol	Chain	Res	Type
1	A	259	LEU
1	A	273	THR
1	A	276	ASP
1	A	277	ILE
1	A	285	HIS
1	A	287	LEU
1	A	294	ASN
1	A	299	ARG
1	A	309	GLU
1	A	313	VAL
1	A	317	GLN
1	A	319	ILE
1	A	324	GLN
1	A	325	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN
1	A	133	ASN
1	A	135	HIS
1	A	136	GLN
1	A	157	GLN
1	A	207	GLN
1	A	217	GLN
1	A	294	ASN
1	A	317	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

1 ligand is 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	DTP	A	338	-	24,32,32	3.97	9 (37%)	32,50,50	1.86	5 (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	DTP	A	338	-	-	0/18/34/34	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	338	DTP	PA-O1A	-11.18	1.10	1.51
2	A	338	DTP	PG-O2G	-8.82	1.23	1.54
2	A	338	DTP	PG-O3G	-7.15	1.29	1.54
2	A	338	DTP	PG-O1G	-6.54	1.29	1.51
2	A	338	DTP	PA-O5'	-2.91	1.45	1.59
2	A	338	DTP	PA-O2A	2.02	1.63	1.54
2	A	338	DTP	O3'-C3'	2.90	1.49	1.43
2	A	338	DTP	C3'-C4'	4.03	1.64	1.53
2	A	338	DTP	PB-O1B	5.51	1.71	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	338	DTP	PA-O3A-PB	-6.40	114.77	132.73
2	A	338	DTP	O3A-PA-O5'	-4.41	91.25	102.94
2	A	338	DTP	O2B-PB-O3B	-2.40	94.20	105.09
2	A	338	DTP	O3G-PG-O1G	-2.24	103.39	110.58
2	A	338	DTP	O3G-PG-O2G	4.23	123.47	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	338	DTP	15	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.