



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:38 PM UTC

PDB ID : 1S76 / pdb_00001s76
Title : T7 RNA polymerase alpha beta methylene ATP elongation complex
Authors : Yin, Y.W.; Steitz, T.A.
Deposited on : 2004-01-29
Resolution : 2.88 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

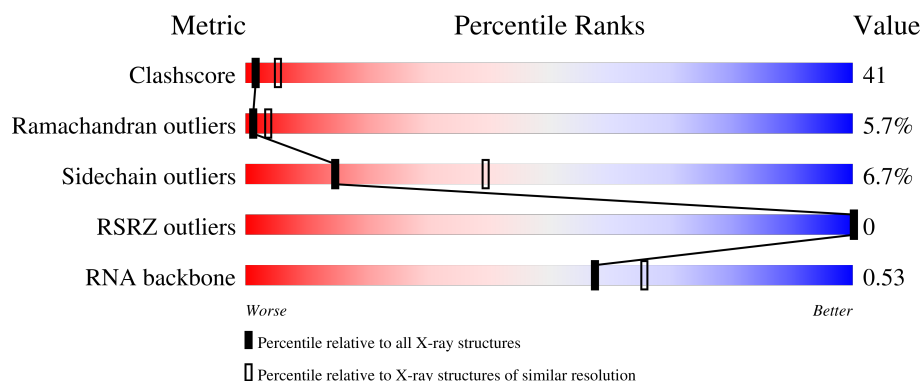
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

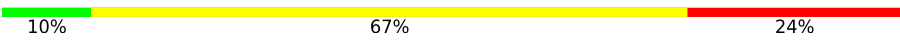
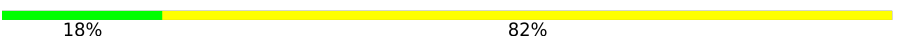
The reported resolution of this entry is 2.88 Å.

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	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)
RNA backbone	3983	1174 (3.10-2.66)

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	T	21	
2	N	17	
3	R	9	
4	D	883	

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
5	APC	R	901	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7561 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 DNA chain called DNA (5'-D(P*GP*CP*CP*GP*TP*GP*CP*GP*CP*AP*TP*TP*CP*GP*CP*CP*GP*TP*GP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	21	Total	C	N	O	P	0	0	0
			429	203	73	132	21			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	17	Total	C	N	O	P	0	0	0
			348	165	60	106	17			

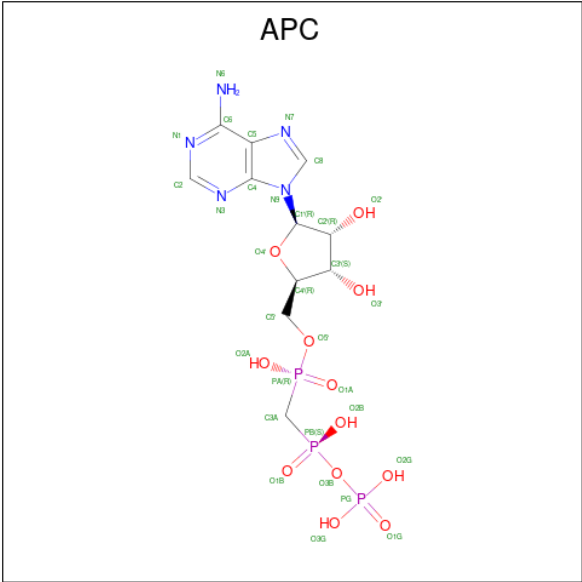
- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*CP*AP*CP*GP*GP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	9	Total	C	N	O	P	0	0	0
			196	87	39	61	9			

- Molecule 4 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	829	Total	C	N	O	S	0	0	0
			6555	4178	1143	1198	36			

- Molecule 5 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	R	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

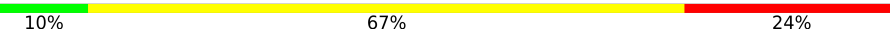
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Mg	0	0
			2	2		

3 Residue-property plots

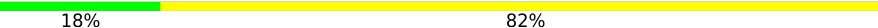
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

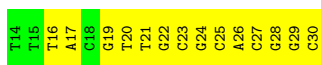
- Molecule 1: DNA (5'-D(P*GP*CP*CP*GP*TP*GP*CP*GP*CP*AP*TP*TP*CP*GP*CP*CP*GP*TP*GP*TP*T)-3')

Chain T: 



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

Chain N: 



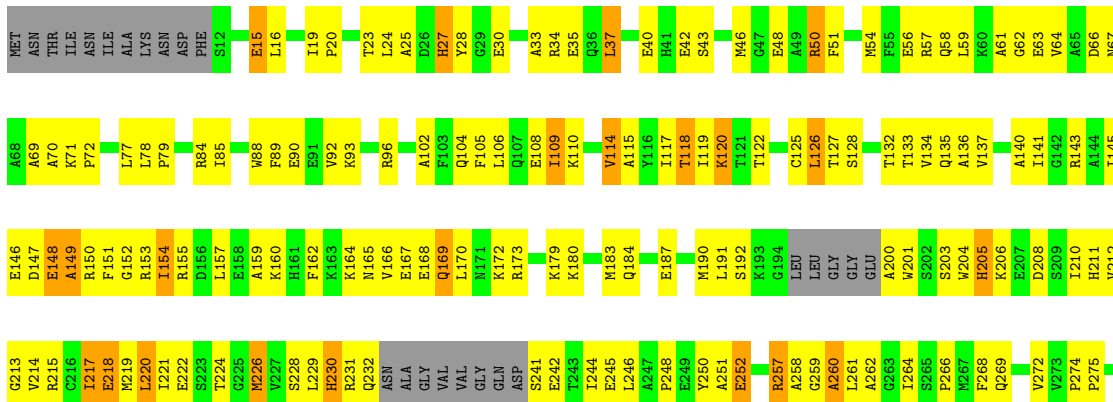
- Molecule 3: RNA (5'-R(P*AP*CP*AP*CP*GP*GP*CP*GP*A)-3')

Chain R: 



- Molecule 4: DNA-directed RNA polymerase

Chain D: 



L870	K793	T729	D660	VAL	F511	P434	E359	W278
R873	T794	F730	S661	VAL	L512	Q435	L360	
F880	V795	D731	K662	THR	A513	G436	P361	I281
A881	V796	G732	K663	VAL	F514	N437	M362	T282
F882	W797	F733	G664	THR	S531	M438	LYS	G283
A883	A798	P734	L665	ASP	L532	D439	PRO	G284
	H799	V735	M666	GLU	L533	M439	GLU	G285
	E800	W736	F667	ASN	P533	L443	ASP	Y286
	R801	Q737	T668	THR	L534	L446	ILE	W287
	Y802	E738	Q669	GLY	A535		ASP	A288
	G803	Y739	P670	GLU	F536		MET	
	I804	K740	N671	ILE	D537	K450	ASN	R292
	S805	K741	Q672	SER	G538	P451	PRO	
	S806	P742	A673	GLU	S539	I452	GLU	L296
		I743	A674	LYS	C540	G453	ALA	V297
	L809	Q744	G675	VAL		G456	LEU	R298
	I810	T745	Y676	LYS	T543		T375	
	H811	R746	Y677	LEU	Q544		A376	K303
	D812	L747	M677	G612	F545	W459	W377	
	S813	N748	L680	T613	F546	L460	K378	R307
	G815	L749	I681	K614	S547	K461		Y308
	T816	M750	W682	A615		I462	E309	D310
	I817	F751	E683	L616	L550	H463		V311
	P818	L752	G684		R551	N466	R366	Y312
		F755	W685	Y623	D552	C467	K367	
		R756	S686	G624	E553	A468	D388	K313
	L824	R757	V689	V625	V554			Y317
	F825	L757		T626	R557	K472	R395	K318
	K826	Q758		T627	A558	W473	L398	A319
	A827	P759	A692	S628	W559	P474	F399	I320
	W828	T760		V629	N560	F475	F400	N321
	R829	I761	A695	T630	L561	P476	M401	
	E830	N762	M696	K631	S564	E477	L402	Q324
	T831	T763	N697	R632		R478	E403	N325
	M832	W764	W698	S633	S564	I479	Q404	
	V833	K765		V634	E565		W328	W328
		D766	S701	M635	T566	N485	E329	
	A843	S767		T636	V667	H486	I330	
	D844	E768	K704	L637		E487	L335	A336
	F845	I769	L705	A638	Y571	N488	V337	A338
	Y846	D770	L706	Y639	V574	A491	F416	
	D847	A771	A707	G640	A575	C492	P417	
	D848		A708	S641	K576		Y418	N339
	F849	E775	E709		K577	S495	N419	
	A850			F644	V578	P496	M420	K343
	D851	T778	D712	G645	N579	L497	D421	W344
	Q852	A779	K713	F646	E580	E498	W422	K345
	L853	P780	T714	R647	I581	N499	R423	
	H854	N781	T715	Q648	L582	T500	G424	V349
	E855	F782	G716	Q649	Q583	W501	R425	E350
	S856	V783	E717	V650	A584	W502	D351	D351
	Q857	H784		L651	D585	A503	Y427	I352
	L858	S785	R720	E652	A586	E504	V428	P353
	D859	Q786	K721	D653	I587	Q505	V429	A354
	K860	D787	R722	T654	N588	D506	S430	I355
	M861	G788	C723	I655	G589	P508	M431	E356
	P862	S789	A724	Q656	T590		F432	R357
	H863	H790	V725	P657			N433	E358
	L864	L791	H726	A658	E593			
		R792		I659				

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	138.72Å 143.32Å 146.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.88 30.00 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.88) 91.2 (30.00-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	14.73 (at 2.90Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.248 , 0.290 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 364.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.29$, $\langle L^2 \rangle = 0.13$	Xtriage
Estimated twinning fraction	0.227 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7561	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: APC, MG

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	T	0.36	0/478	0.89	7/734 (1.0%)
2	N	0.33	0/388	0.58	0/595
3	R	0.43	0/219	0.65	0/338
4	D	0.44	4/6706 (0.1%)	0.96	32/9068 (0.4%)
All	All	0.43	4/7791 (0.1%)	0.93	39/10735 (0.4%)

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	T	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	251	ALA	C-N	9.73	1.47	1.34
4	D	766	ASP	C-N	-7.74	1.22	1.33
4	D	252	GLU	C-N	-5.14	1.26	1.33
4	D	292	ARG	C-N	-5.00	1.22	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	423	ARG	N-CA-C	-10.62	100.31	113.38
4	D	461	LYS	N-CA-C	-9.51	100.90	111.07
4	D	717	GLU	N-CA-C	-8.61	98.93	110.55
4	D	828	VAL	N-CA-C	-8.44	97.48	109.63
4	D	860	LYS	N-CA-C	-7.50	103.69	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	502	TRP	N-CA-C	-7.10	103.55	111.71
4	D	535	ALA	N-CA-C	6.92	119.84	109.25
4	D	433	ASN	N-CA-C	6.74	114.28	108.22
4	D	733	PHE	CA-C-N	6.20	126.41	119.90
4	D	733	PHE	C-N-CA	6.20	126.41	119.90
1	T	117	DG	C5'-C4'-C3'	-6.07	105.79	114.90
1	T	118	DC	C5'-C4'-C3'	-5.91	106.03	114.90
4	D	359	GLU	CB-CA-C	-5.88	109.81	116.63
4	D	409	ALA	N-CA-C	-5.82	102.85	110.53
4	D	84	ARG	N-CA-C	-5.79	106.85	114.31
4	D	824	LEU	N-CA-C	-5.79	105.11	111.82
4	D	560	ASN	N-CA-C	5.74	119.34	111.54
4	D	345	LYS	N-CA-C	-5.69	104.77	110.97
4	D	428	ALA	N-CA-C	-5.66	102.52	110.50
4	D	220	LEU	N-CA-C	-5.64	104.75	111.69
4	D	833	VAL	N-CA-C	5.60	115.73	110.30
4	D	673	ALA	N-CA-C	-5.59	105.95	112.89
4	D	217	ILE	N-CA-C	-5.58	104.93	110.62
4	D	815	GLY	N-CA-C	5.46	119.26	110.90
4	D	487	GLU	N-CA-C	5.42	117.19	111.28
4	D	127	THR	N-CA-C	-5.41	106.16	114.16
1	T	120	DT	C5'-C4'-C3'	-5.37	106.85	114.90
1	T	119	DT	C5'-C4'-C3'	-5.35	106.87	114.90
4	D	313	MET	CA-C-N	5.31	124.76	119.24
4	D	313	MET	C-N-CA	5.31	124.76	119.24
4	D	460	LEU	N-CA-C	-5.29	99.53	110.80
4	D	452	ILE	N-CA-C	5.22	115.66	110.23
1	T	118	DC	C4'-C3'-O3'	5.21	117.82	110.00
4	D	479	ILE	N-CA-C	-5.17	105.35	110.62
4	D	674	ALA	N-CA-C	-5.10	106.75	113.12
4	D	343	LYS	N-CA-C	-5.07	105.41	112.45
1	T	117	DG	C4'-C3'-O3'	5.05	117.57	110.00
4	D	218	GLU	N-CA-C	-5.05	103.38	110.35
1	T	116	DC	C5'-C4'-C3'	-5.02	107.37	114.90

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	T	116	DC	Sidechain
1	T	117	DG	Sidechain
1	T	118	DC	Sidechain

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Mol	Chain	Res	Type	Group
1	T	119	DT	Sidechain
1	T	120	DT	Sidechain

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	T	429	0	238	29	0
2	N	348	0	193	28	0
3	R	196	0	100	15	0
4	D	6555	0	6519	551	0
5	R	31	0	14	11	0
6	D	2	0	0	0	0
All	All	7561	0	7064	605	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 41.

All (605) 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)
3:R:2:A:O3'	5:R:901:APC:H5'1	1.34	1.28
4:D:759:PRO:HG2	4:D:764:ASN:ND2	1.61	1.15
4:D:763:THR:O	4:D:764:ASN:CG	1.96	1.08
4:D:724:ALA:HB2	4:D:738:GLU:HB3	1.36	1.06
3:R:2:A:O3'	5:R:901:APC:C5'	2.09	1.01
4:D:417:PRO:HG2	4:D:429:VAL:HB	1.48	0.96
4:D:278:TRP:H	4:D:321:ASN:HD21	0.98	0.95
4:D:798:ALA:HB1	4:D:804:ILE:HD12	1.49	0.94
4:D:360:LEU:H	4:D:361:PRO:HD2	1.30	0.94
4:D:109:ILE:HG23	4:D:150:ARG:H	1.31	0.93
2:N:16:DT:O3'	4:D:378:LYS:HD3	1.69	0.93
4:D:349:VAL:HG22	4:D:503:ALA:HB1	1.51	0.92
2:N:27:DC:H1'	2:N:28:DG:H5''	1.52	0.91
4:D:763:THR:O	4:D:764:ASN:OD1	1.88	0.90
4:D:162:PHE:HA	4:D:166:VAL:HB	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:756:ARG:H	4:D:756:ARG:HE	1.20	0.88
4:D:755:PHE:HA	4:D:756:ARG:HH21	1.38	0.87
4:D:72:PRO:HG3	4:D:257:ARG:HG3	1.56	0.86
4:D:746:ARG:HG3	4:D:756:ARG:HG3	1.56	0.86
1:T:120:DT:H2''	1:T:119:DT:OP2	1.76	0.85
4:D:756:ARG:HE	4:D:756:ARG:N	1.74	0.85
4:D:450:LYS:HE2	4:D:817:ILE:HD11	1.56	0.85
4:D:856:SER:O	4:D:857:GLN:HB3	1.77	0.84
1:T:116:DC:H2''	1:T:115:DC:OP2	1.77	0.84
4:D:759:PRO:CG	4:D:764:ASN:ND2	2.38	0.84
1:T:124:DC:N4	2:N:24:DG:H1	1.76	0.83
4:D:473:VAL:HG22	4:D:474:PRO:HD2	1.61	0.83
3:R:5:G:H2'	3:R:4:C:H6	1.42	0.82
4:D:152:GLY:HA2	4:D:155:ARG:HD3	1.61	0.82
4:D:126:LEU:HA	4:D:132:THR:HG21	1.60	0.82
4:D:584:ALA:HB1	4:D:587:ILE:HG23	1.62	0.81
2:N:17:DA:P	4:D:378:LYS:HD3	2.19	0.81
4:D:358:GLU:OE1	4:D:387:LYS:HD2	1.81	0.81
4:D:461:LYS:HD2	4:D:479:ILE:HG23	1.62	0.81
4:D:724:ALA:CB	4:D:738:GLU:HB3	2.11	0.81
4:D:433:ASN:HD22	4:D:435:GLN:H	1.28	0.80
4:D:559:VAL:HG23	4:D:561:LEU:HD13	1.61	0.80
4:D:278:TRP:H	4:D:321:ASN:ND2	1.79	0.80
4:D:759:PRO:CB	4:D:764:ASN:HD21	1.96	0.79
4:D:861:MET:HE3	4:D:862:PRO:HD2	1.61	0.79
4:D:386:ARG:HD3	4:D:387:LYS:N	1.97	0.79
4:D:873:ARG:HG3	4:D:873:ARG:HH11	1.47	0.78
1:T:124:DC:H42	2:N:24:DG:H1	1.29	0.78
4:D:120:LYS:HE2	4:D:752:LEU:HD23	1.66	0.78
4:D:651:LEU:CD1	4:D:670:PRO:HB2	2.13	0.78
4:D:67:ASN:HD22	4:D:69:ALA:H	1.30	0.78
4:D:623:TYR:HB2	4:D:666:MET:HE1	1.66	0.78
4:D:630:THR:O	4:D:634:VAL:HG23	1.84	0.77
4:D:662:GLY:O	4:D:665:LEU:HD22	1.83	0.77
4:D:759:PRO:CG	4:D:764:ASN:HD21	1.97	0.77
4:D:213:GLY:O	4:D:217:ILE:HG12	1.85	0.76
2:N:23:DC:H2''	2:N:24:DG:H5'	1.68	0.76
4:D:826:LYS:O	4:D:830:GLU:HG3	1.85	0.75
4:D:846:TYR:HA	4:D:849:PHE:CE1	2.22	0.75
3:R:2:A:H2'	5:R:901:APC:H8	1.67	0.75
4:D:23:THR:O	4:D:27:HIS:HB2	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:473:VAL:CG2	4:D:474:PRO:HD2	2.17	0.74
4:D:663:LYS:H	4:D:663:LYS:HD2	1.50	0.74
4:D:705:LEU:HD22	4:D:858:LEU:HD22	1.69	0.74
2:N:20:DT:H2''	2:N:21:DT:H72	1.70	0.74
3:R:5:G:H2'	3:R:4:C:C6	2.21	0.73
4:D:550:LEU:HD11	4:D:695:ALA:HB2	1.69	0.73
4:D:154:ILE:HG22	4:D:162:PHE:HB2	1.70	0.72
4:D:190:MET:HE3	4:D:191:LEU:H	1.52	0.72
4:D:109:ILE:HG21	4:D:148:GLU:HB3	1.71	0.72
4:D:298:ARG:NE	4:D:419:ASN:HD21	1.87	0.72
4:D:689:VAL:HG12	4:D:692:ALA:HB3	1.70	0.72
4:D:359:GLU:HB3	4:D:361:PRO:HD2	1.71	0.72
4:D:584:ALA:HB1	4:D:587:ILE:CG2	2.19	0.72
4:D:828:VAL:O	4:D:829:ARG:HB2	1.88	0.72
4:D:261:LEU:O	4:D:264:ILE:HG13	1.89	0.72
4:D:335:LEU:HD22	4:D:339:ASN:ND2	2.05	0.72
4:D:125:CYS:O	4:D:132:THR:HG22	1.90	0.71
4:D:651:LEU:HD11	4:D:670:PRO:HB2	1.71	0.71
4:D:631:LYS:HD2	4:D:632:ARG:N	2.05	0.71
4:D:78:LEU:HB3	4:D:79:PRO:HD3	1.73	0.71
4:D:577:LYS:HE3	4:D:577:LYS:HA	1.73	0.71
4:D:639:TYR:CE1	4:D:783:VAL:HG21	2.26	0.71
4:D:495:SER:HB3	4:D:498:GLU:HB2	1.73	0.70
4:D:456:GLY:O	4:D:459:TRP:O	2.09	0.70
4:D:655:ILE:HD12	4:D:674:ALA:HB2	1.72	0.70
4:D:766:ASP:O	4:D:767:SER:HB2	1.92	0.69
4:D:42:GLU:HG2	4:D:46:MET:HE2	1.75	0.69
4:D:864:LEU:HD12	4:D:864:LEU:H	1.56	0.69
3:R:2:A:O2'	5:R:901:APC:O4'	2.10	0.69
4:D:154:ILE:HD12	4:D:154:ILE:H	1.56	0.69
4:D:756:ARG:H	4:D:756:ARG:NE	1.91	0.69
4:D:806:SER:O	4:D:816:THR:HG23	1.92	0.69
4:D:565:GLU:OE2	4:D:566:THR:HG22	1.93	0.68
2:N:19:DG:H1'	2:N:20:DT:H73	1.74	0.68
4:D:360:LEU:H	4:D:361:PRO:CD	2.04	0.68
4:D:574:VAL:O	4:D:578:VAL:HG23	1.93	0.68
4:D:629:VAL:HG12	4:D:630:THR:H	1.59	0.68
4:D:308:TYR:HA	4:D:311:VAL:HG13	1.76	0.68
4:D:298:ARG:HE	4:D:419:ASN:HD21	1.40	0.68
4:D:419:ASN:HD22	4:D:419:ASN:C	2.01	0.68
4:D:466:ASN:HD21	4:D:478:ARG:HH11	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:126:LEU:HA	4:D:132:THR:CG2	2.24	0.68
4:D:85:ILE:HA	4:D:219:MET:CE	2.23	0.68
4:D:298:ARG:HE	4:D:419:ASN:ND2	1.91	0.68
4:D:360:LEU:N	4:D:361:PRO:HD2	2.07	0.68
4:D:109:ILE:HD13	4:D:114:VAL:HG22	1.76	0.68
4:D:117:ILE:HG12	4:D:752:LEU:HD22	1.75	0.68
4:D:433:ASN:ND2	4:D:435:GLN:HB2	2.09	0.68
4:D:500:THR:O	4:D:501:TRP:HB3	1.94	0.67
4:D:46:MET:HE1	4:D:269:GLN:CD	2.20	0.67
4:D:829:ARG:NH2	4:D:882:PHE:H	1.93	0.67
4:D:853:LEU:HD12	4:D:853:LEU:H	1.60	0.67
4:D:631:LYS:HD2	4:D:631:LYS:C	2.20	0.67
4:D:109:ILE:HG23	4:D:150:ARG:N	2.08	0.67
4:D:278:TRP:CD2	4:D:284:GLY:HA3	2.30	0.67
4:D:154:ILE:HD12	4:D:154:ILE:N	2.09	0.67
4:D:726:HIS:HD2	4:D:735:VAL:O	1.78	0.67
4:D:828:VAL:HG21	4:D:883:ALA:HA	1.77	0.66
2:N:27:DC:H2''	2:N:28:DG:C5'	2.25	0.66
4:D:219:MET:HA	4:D:222:GLU:HB2	1.77	0.66
4:D:88:TRP:CZ2	4:D:215:ARG:HD3	2.31	0.66
4:D:423:ARG:NH1	4:D:423:ARG:HB2	2.11	0.65
4:D:873:ARG:HG3	4:D:873:ARG:NH1	2.11	0.65
4:D:589:GLY:HA2	4:D:614:LYS:H	1.60	0.65
4:D:438:ASP:OD2	4:D:508:PRO:HG2	1.97	0.65
4:D:362:MET:C	4:D:381:ALA:HB2	2.22	0.65
4:D:581:ILE:HG21	4:D:680:LEU:HD22	1.80	0.64
4:D:210:ILE:O	4:D:214:VAL:HG23	1.98	0.64
4:D:40:GLU:CD	4:D:286:TYR:HB3	2.22	0.64
4:D:208:ASP:O	4:D:212:VAL:HG23	1.97	0.64
4:D:307:ARG:HG2	4:D:736:TRP:CZ3	2.32	0.64
4:D:281:ILE:HG12	4:D:282:THR:HG23	1.80	0.64
4:D:378:LYS:C	4:D:378:LYS:HD2	2.22	0.64
4:D:534:LEU:HD12	4:D:818:PRO:HA	1.78	0.64
4:D:663:LYS:HD2	4:D:663:LYS:N	2.13	0.64
4:D:151:PHE:C	4:D:153:ARG:H	2.06	0.63
4:D:439:MET:HE3	4:D:443:LEU:CD2	2.28	0.63
4:D:576:LYS:HZ1	4:D:576:LYS:HA	1.64	0.63
4:D:767:SER:O	4:D:768:GLU:HB3	1.98	0.63
4:D:639:TYR:HE1	4:D:783:VAL:HG21	1.63	0.63
4:D:701:SER:HB2	4:D:861:MET:HE1	1.81	0.62
4:D:854:HIS:O	4:D:858:LEU:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:124:DC:H1'	1:T:123:DG:H5'	1.80	0.62
4:D:104:GLN:HE21	4:D:104:GLN:HA	1.63	0.62
3:R:2:A:C3'	5:R:901:APC:H5'1	2.28	0.62
4:D:861:MET:HE3	4:D:862:PRO:CD	2.30	0.62
4:D:204:TRP:O	4:D:208:ASP:HB2	1.99	0.62
4:D:218:GLU:C	4:D:220:LEU:H	2.07	0.62
4:D:810:ILE:HB	4:D:813:SER:HB3	1.82	0.62
4:D:122:THR:HG22	4:D:141:ILE:HD11	1.81	0.62
1:T:117:DG:H5''	4:D:421:ASP:HB2	1.81	0.62
4:D:828:VAL:O	4:D:829:ARG:CB	2.47	0.61
4:D:488:ASN:HB3	4:D:501:TRP:CZ3	2.35	0.61
4:D:117:ILE:HG23	4:D:752:LEU:HD21	1.82	0.61
4:D:85:ILE:HA	4:D:219:MET:HE1	1.83	0.61
4:D:473:VAL:HG21	4:D:477:GLU:OE1	2.00	0.61
4:D:473:VAL:HG21	4:D:477:GLU:CD	2.25	0.61
4:D:565:GLU:HG2	4:D:566:THR:N	2.15	0.61
4:D:298:ARG:CZ	4:D:419:ASN:HD21	2.14	0.61
4:D:46:MET:HE1	4:D:269:GLN:NE2	2.16	0.60
4:D:720:ARG:HH12	4:D:854:HIS:HA	1.67	0.60
4:D:359:GLU:O	4:D:360:LEU:HG	2.02	0.60
4:D:546:PHE:CE2	4:D:638:ALA:HB1	2.36	0.60
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.37	0.60
4:D:298:ARG:NH2	4:D:419:ASN:HD21	1.98	0.60
4:D:579:ASN:HA	4:D:582:LEU:HD12	1.83	0.60
4:D:50:ARG:HG3	4:D:51:PHE:N	2.16	0.60
4:D:729:THR:OG1	4:D:733:PHE:HB3	2.01	0.60
4:D:706:LEU:HD12	4:D:725:VAL:HG12	1.83	0.60
4:D:743:ILE:HD12	4:D:744:GLN:H	1.66	0.60
2:N:24:DG:H2''	2:N:25:DC:C5	2.37	0.59
4:D:70:ALA:C	4:D:72:PRO:HD2	2.26	0.59
4:D:71:LYS:N	4:D:72:PRO:HD2	2.17	0.59
4:D:747:LEU:HD23	4:D:747:LEU:N	2.18	0.59
4:D:576:LYS:HA	4:D:576:LYS:NZ	2.17	0.59
4:D:48:GLU:HG2	4:D:262:ALA:C	2.26	0.59
4:D:118:THR:O	4:D:122:THR:HG23	2.03	0.59
4:D:169:GLN:H	4:D:169:GLN:NE2	2.00	0.59
4:D:230:HIS:O	4:D:231:ARG:HG3	2.02	0.59
4:D:423:ARG:HB2	4:D:423:ARG:HH11	1.68	0.59
4:D:349:VAL:HG22	4:D:503:ALA:CB	2.30	0.58
4:D:629:VAL:C	4:D:631:LYS:H	2.11	0.58
4:D:43:SER:HA	4:D:46:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:663:LYS:H	4:D:663:LYS:CD	2.16	0.58
4:D:784:HIS:HA	4:D:787:ASP:OD2	2.03	0.58
4:D:421:ASP:O	4:D:422:TRP:HB3	2.03	0.58
4:D:88:TRP:O	4:D:92:VAL:HG23	2.04	0.58
4:D:452:ILE:HG23	4:D:453:GLY:N	2.19	0.58
4:D:463:HIS:HB2	4:D:534:LEU:HD22	1.85	0.58
4:D:567:VAL:HB	4:D:880:PHE:CD1	2.39	0.58
1:T:120:DT:H5'	4:D:641:SER:HA	1.86	0.57
4:D:551:ARG:O	4:D:870:LEU:HB3	2.04	0.57
4:D:731:ASP:HB3	4:D:793:LYS:HD2	1.84	0.57
4:D:755:PHE:HA	4:D:756:ARG:NH2	2.15	0.57
4:D:54:MET:HA	4:D:57:ARG:HG3	1.86	0.57
4:D:54:MET:O	4:D:57:ARG:HG3	2.04	0.57
4:D:143:ARG:HH21	4:D:206:LYS:HG2	1.67	0.57
4:D:544:GLN:HG2	4:D:559:VAL:HB	1.86	0.57
2:N:28:DG:H2''	2:N:29:DG:N7	2.19	0.57
4:D:25:ALA:C	4:D:27:HIS:H	2.11	0.57
4:D:126:LEU:HD22	4:D:246:LEU:HD23	1.86	0.57
4:D:150:ARG:NE	4:D:150:ARG:HA	2.19	0.57
4:D:759:PRO:HG2	4:D:764:ASN:HD22	1.61	0.57
2:N:17:DA:OP1	4:D:378:LYS:CD	2.53	0.57
4:D:125:CYS:HA	4:D:128:SER:OG	2.04	0.57
2:N:27:DC:C1'	2:N:28:DG:H5''	2.30	0.57
4:D:85:ILE:HA	4:D:219:MET:HE2	1.87	0.57
4:D:115:ALA:O	4:D:118:THR:HB	2.04	0.57
4:D:495:SER:CB	4:D:498:GLU:HB2	2.33	0.57
4:D:565:GLU:CG	4:D:566:THR:H	2.18	0.57
4:D:712:ASP:O	4:D:716:GLY:HA2	2.05	0.57
4:D:741:LYS:HD2	4:D:768:GLU:OE1	2.05	0.56
4:D:154:ILE:CG2	4:D:162:PHE:HB2	2.34	0.56
4:D:226:MET:HA	4:D:250:TYR:HD1	1.71	0.56
4:D:228:SER:HB2	4:D:245:GLU:CG	2.36	0.56
4:D:540:CYS:O	4:D:544:GLN:HG3	2.04	0.56
4:D:571:TYR:HD2	4:D:627:ARG:NH2	2.03	0.56
4:D:155:ARG:H	4:D:155:ARG:HD2	1.69	0.56
4:D:308:TYR:CE2	4:D:734:PRO:HG2	2.41	0.56
4:D:613:THR:HG23	4:D:676:TYR:CE1	2.41	0.56
4:D:629:VAL:O	4:D:631:LYS:N	2.36	0.56
4:D:219:MET:H	4:D:222:GLU:HG3	1.69	0.56
4:D:423:ARG:HD2	4:D:781:ASN:ND2	2.21	0.56
2:N:19:DG:H21	4:D:670:PRO:HD2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:183:MET:HE3	4:D:187:GLU:HB2	1.88	0.55
4:D:816:THR:OG1	4:D:824:LEU:HD22	2.05	0.55
4:D:61:ALA:O	4:D:63:GLU:HG3	2.07	0.55
4:D:473:VAL:HG22	4:D:474:PRO:CD	2.34	0.55
4:D:105:PHE:HB3	4:D:204:TRP:CZ3	2.40	0.55
4:D:298:ARG:HB2	4:D:421:ASP:HA	1.88	0.55
4:D:468:ALA:HA	4:D:505:GLN:HB3	1.89	0.55
4:D:109:ILE:HD12	4:D:109:ILE:H	1.72	0.55
4:D:725:VAL:HG23	4:D:737:GLN:HB3	1.88	0.55
4:D:400:PHE:HA	4:D:403:GLU:OE2	2.07	0.55
4:D:589:GLY:HA2	4:D:613:THR:HB	1.88	0.55
4:D:725:VAL:CG2	4:D:737:GLN:HB3	2.36	0.55
4:D:752:LEU:H	4:D:752:LEU:HD12	1.71	0.55
4:D:419:ASN:C	4:D:419:ASN:ND2	2.64	0.55
4:D:472:LYS:HB2	4:D:472:LYS:NZ	2.21	0.55
4:D:48:GLU:HG2	4:D:262:ALA:O	2.07	0.55
4:D:69:ALA:HA	4:D:257:ARG:HD2	1.89	0.55
4:D:143:ARG:NH2	4:D:206:LYS:HG2	2.22	0.55
4:D:852:GLN:O	4:D:853:LEU:C	2.50	0.55
1:T:115:DC:H2''	1:T:114:DG:H5'	1.88	0.55
4:D:855:GLU:CD	4:D:856:SER:H	2.14	0.55
1:T:120:DT:C4	4:D:636:THR:HG21	2.41	0.54
2:N:22:DG:H2''	2:N:23:DC:C5	2.41	0.54
4:D:565:GLU:CG	4:D:566:THR:N	2.69	0.54
1:T:119:DT:H2''	1:T:118:DC:OP2	2.07	0.54
1:T:115:DC:H4'	4:D:431:MET:HE3	1.89	0.54
4:D:500:THR:O	4:D:501:TRP:CB	2.55	0.54
4:D:218:GLU:O	4:D:219:MET:HB2	2.07	0.54
4:D:409:ALA:O	4:D:410:ASN:HB2	2.08	0.54
4:D:416:PHE:CZ	4:D:434:PRO:HD3	2.43	0.54
4:D:146:GLU:C	4:D:148:GLU:H	2.14	0.54
4:D:190:MET:CE	4:D:191:LEU:H	2.21	0.54
4:D:309:GLU:HG3	4:D:310:ASP:OD1	2.07	0.54
4:D:543:ILE:HB	4:D:559:VAL:HG11	1.89	0.54
2:N:27:DC:H2''	2:N:28:DG:O5'	2.08	0.54
4:D:579:ASN:HD22	4:D:582:LEU:HD12	1.72	0.54
4:D:40:GLU:OE2	4:D:288:ALA:HB3	2.08	0.54
4:D:298:ARG:HH21	4:D:419:ASN:HD21	1.56	0.54
4:D:28:TYR:CZ	4:D:274:PRO:HD2	2.43	0.53
4:D:433:ASN:HD22	4:D:435:GLN:N	2.01	0.53
4:D:534:LEU:CD1	4:D:818:PRO:HA	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:757:LEU:HD23	4:D:758:GLN:N	2.24	0.53
4:D:110:LYS:O	4:D:114:VAL:HG23	2.08	0.53
4:D:668:THR:O	4:D:669:GLN:HB3	2.08	0.53
4:D:740:LYS:HD3	4:D:769:ILE:HA	1.90	0.53
4:D:796:VAL:O	4:D:800:GLU:HG3	2.08	0.53
2:N:20:DT:H2''	2:N:21:DT:C7	2.37	0.53
3:R:4:C:O2'	3:R:3:G:H5'	2.09	0.53
4:D:613:THR:O	4:D:616:LEU:N	2.35	0.53
4:D:629:VAL:HG12	4:D:630:THR:N	2.21	0.53
4:D:855:GLU:O	4:D:856:SER:HB2	2.08	0.53
4:D:133:THR:HG23	4:D:136:ALA:H	1.72	0.53
4:D:612:GLY:O	4:D:616:LEU:HB2	2.09	0.53
4:D:748:ASN:O	4:D:749:LEU:HD23	2.08	0.53
4:D:759:PRO:CB	4:D:764:ASN:ND2	2.65	0.53
3:R:2:A:H2'	5:R:901:APC:C8	2.35	0.53
4:D:228:SER:C	4:D:229:LEU:HD22	2.34	0.53
4:D:466:ASN:HD21	4:D:478:ARG:NH1	2.07	0.53
4:D:585:ASP:O	4:D:586:ALA:CB	2.57	0.53
4:D:746:ARG:HD3	4:D:746:ARG:N	2.22	0.53
4:D:162:PHE:CE1	4:D:167:GLU:HB2	2.43	0.53
4:D:468:ALA:HB2	4:D:511:PHE:CE1	2.44	0.53
4:D:585:ASP:O	4:D:586:ALA:HB2	2.08	0.53
4:D:852:GLN:OE1	4:D:853:LEU:HB2	2.08	0.53
4:D:852:GLN:OE1	4:D:853:LEU:HD13	2.09	0.53
4:D:169:GLN:NE2	4:D:169:GLN:N	2.56	0.53
4:D:416:PHE:CE2	4:D:434:PRO:HD3	2.43	0.52
2:N:27:DC:H1'	2:N:28:DG:OP1	2.08	0.52
4:D:77:LEU:HD22	4:D:224:THR:HB	1.91	0.52
4:D:180:LYS:HA	4:D:751:PHE:CE1	2.45	0.52
4:D:613:THR:O	4:D:614:LYS:C	2.52	0.52
4:D:360:LEU:N	4:D:361:PRO:CD	2.70	0.52
4:D:791:LEU:HD21	4:D:809:LEU:HD13	1.92	0.52
4:D:264:ILE:O	4:D:264:ILE:HD12	2.08	0.52
4:D:421:ASP:OD1	4:D:423:ARG:NH1	2.37	0.52
4:D:104:GLN:HA	4:D:104:GLN:NE2	2.24	0.52
4:D:538:GLY:HA3	4:D:883:ALA:HB3	1.91	0.52
4:D:881:ALA:O	4:D:882:PHE:HB2	2.09	0.52
4:D:298:ARG:HE	4:D:419:ASN:CG	2.18	0.52
4:D:704:LYS:HB2	4:D:775:GLU:OE2	2.09	0.52
4:D:743:ILE:CD1	4:D:744:GLN:H	2.23	0.52
4:D:152:GLY:CA	4:D:155:ARG:HD3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:550:LEU:HD11	4:D:695:ALA:CB	2.38	0.52
4:D:85:ILE:HD13	4:D:219:MET:SD	2.49	0.52
4:D:155:ARG:H	4:D:155:ARG:CD	2.23	0.52
4:D:141:ILE:O	4:D:145:ILE:HG12	2.10	0.52
4:D:750:MET:HE3	4:D:750:MET:N	2.22	0.52
4:D:763:THR:C	4:D:764:ASN:CG	2.74	0.52
4:D:696:MET:HE3	4:D:697:ASN:ND2	2.25	0.52
4:D:810:ILE:O	4:D:811:HIS:HB2	2.09	0.52
4:D:147:ASP:O	4:D:148:GLU:HG2	2.10	0.51
4:D:665:LEU:HD23	4:D:665:LEU:H	1.74	0.51
4:D:791:LEU:O	4:D:795:VAL:HG23	2.11	0.51
4:D:102:ALA:O	4:D:106:LEU:HB2	2.10	0.51
4:D:228:SER:HB2	4:D:245:GLU:HG3	1.92	0.51
4:D:655:ILE:CD1	4:D:674:ALA:HB2	2.40	0.51
4:D:671:ASN:C	4:D:673:ALA:H	2.18	0.51
4:D:655:ILE:HG21	4:D:670:PRO:HB3	1.90	0.51
4:D:151:PHE:O	4:D:153:ARG:HG3	2.10	0.51
4:D:278:TRP:CE2	4:D:284:GLY:HA3	2.45	0.51
4:D:750:MET:HE3	4:D:750:MET:H	1.75	0.51
4:D:248:PRO:O	4:D:252:GLU:HG3	2.10	0.51
4:D:707:ALA:O	4:D:722:ARG:HG2	2.10	0.51
4:D:421:ASP:O	4:D:422:TRP:CB	2.58	0.51
4:D:565:GLU:CD	4:D:566:THR:H	2.18	0.51
4:D:856:SER:O	4:D:857:GLN:CB	2.53	0.51
4:D:24:LEU:O	4:D:28:TYR:N	2.39	0.51
4:D:85:ILE:HD13	4:D:219:MET:CE	2.41	0.51
4:D:731:ASP:OD2	4:D:792:ARG:NE	2.43	0.51
4:D:308:TYR:HE2	4:D:734:PRO:HG2	1.75	0.50
4:D:459:TRP:O	4:D:534:LEU:HD11	2.11	0.50
4:D:613:THR:O	4:D:615:ALA:N	2.45	0.50
4:D:67:ASN:ND2	4:D:69:ALA:H	2.03	0.50
4:D:343:LYS:HA	4:D:355:ILE:HD11	1.94	0.50
4:D:398:LEU:C	4:D:398:LEU:HD23	2.36	0.50
4:D:492:CYS:HB3	4:D:502:TRP:CD1	2.47	0.50
4:D:698:TRP:HZ3	4:D:845:PHE:HD2	1.58	0.50
2:N:17:DA:P	4:D:378:LYS:CD	2.98	0.50
2:N:26:DA:H2"	2:N:27:DC:C6	2.46	0.50
4:D:108:GLU:O	4:D:150:ARG:HB2	2.11	0.50
4:D:266:PRO:HG2	4:D:268:PHE:CZ	2.46	0.50
4:D:547:SER:HA	4:D:552:ASP:HB3	1.94	0.50
4:D:303:LYS:HE2	4:D:303:LYS:H	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:GLU:HG2	4:D:272:VAL:HG21	1.92	0.50
4:D:307:ARG:HG2	4:D:736:TRP:CE3	2.47	0.50
4:D:655:ILE:O	4:D:659:ILE:HG12	2.12	0.50
4:D:308:TYR:HA	4:D:311:VAL:CG1	2.40	0.50
4:D:623:TYR:CB	4:D:666:MET:HE1	2.40	0.50
4:D:720:ARG:NH1	4:D:854:HIS:HA	2.26	0.50
4:D:816:THR:HG22	4:D:817:ILE:H	1.76	0.50
4:D:554:VAL:O	4:D:557:ARG:HB3	2.11	0.50
5:R:901:APC:H3A1	5:R:901:APC:H3'	1.94	0.50
4:D:551:ARG:C	4:D:870:LEU:HB3	2.37	0.49
4:D:766:ASP:O	4:D:767:SER:CB	2.57	0.49
4:D:378:LYS:HD2	4:D:378:LYS:O	2.13	0.49
4:D:218:GLU:C	4:D:220:LEU:N	2.71	0.49
4:D:357:ARG:HG2	4:D:357:ARG:HH11	1.77	0.49
4:D:57:ARG:HH11	4:D:57:ARG:HG2	1.78	0.49
4:D:126:LEU:HD22	4:D:246:LEU:CD2	2.43	0.49
4:D:155:ARG:HG3	4:D:162:PHE:CE2	2.48	0.49
4:D:630:THR:HA	4:D:681:ILE:HD13	1.95	0.49
4:D:855:GLU:OE1	4:D:856:SER:N	2.45	0.49
3:R:2:A:C2'	5:R:901:APC:O4'	2.61	0.49
4:D:353:PRO:HD2	4:D:398:LEU:CD1	2.43	0.49
1:T:122:DC:H2''	1:T:121:DA:OP2	2.12	0.49
4:D:724:ALA:HB2	4:D:738:GLU:CB	2.25	0.49
4:D:565:GLU:HG2	4:D:566:THR:H	1.75	0.49
4:D:855:GLU:CD	4:D:856:SER:N	2.71	0.49
4:D:613:THR:HG22	4:D:614:LYS:N	2.27	0.48
4:D:709:GLU:HB2	4:D:722:ARG:HG3	1.95	0.48
1:T:130:DG:H2''	1:T:129:DC:H5	1.78	0.48
4:D:645:GLY:O	4:D:649:GLN:HG3	2.14	0.48
2:N:22:DG:H2''	2:N:23:DC:H5	1.78	0.48
4:D:66:ASP:O	4:D:71:LYS:NZ	2.44	0.48
4:D:151:PHE:C	4:D:153:ARG:N	2.71	0.48
4:D:423:ARG:HH21	4:D:784:HIS:CD2	2.31	0.48
4:D:433:ASN:C	4:D:435:GLN:H	2.22	0.48
3:R:9:C:H5'	4:D:746:ARG:HH22	1.78	0.48
4:D:120:LYS:HE2	4:D:752:LEU:HB3	1.96	0.48
4:D:828:VAL:CG2	4:D:883:ALA:HA	2.44	0.48
4:D:257:ARG:O	4:D:260:ALA:HB3	2.14	0.48
4:D:557:ARG:HH12	4:D:564:SER:HB2	1.79	0.48
4:D:756:ARG:O	4:D:757:LEU:HB2	2.14	0.48
4:D:631:LYS:HE3	4:D:635:MET:HE3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:231:ARG:HA	4:D:242:GLU:OE1	2.13	0.48
4:D:488:ASN:HB3	4:D:501:TRP:CE3	2.49	0.48
4:D:590:THR:H	4:D:613:THR:HB	1.79	0.48
4:D:586:ALA:H	4:D:589:GLY:H	1.62	0.48
4:D:783:VAL:O	4:D:786:GLN:HB2	2.14	0.48
1:T:126:DT:H1'	1:T:125:DG:H5''	1.96	0.48
4:D:729:THR:HG1	4:D:733:PHE:HB3	1.78	0.48
4:D:744:GLN:HB3	4:D:757:LEU:H	1.79	0.48
4:D:798:ALA:O	4:D:802:TYR:HB2	2.14	0.48
4:D:122:THR:O	4:D:126:LEU:HB2	2.14	0.47
4:D:298:ARG:HH21	4:D:419:ASN:ND2	2.11	0.47
4:D:761:ILE:O	4:D:763:THR:N	2.46	0.47
4:D:109:ILE:H	4:D:109:ILE:CD1	2.25	0.47
4:D:790:HIS:ND1	4:D:831:THR:HG22	2.29	0.47
4:D:446:LEU:O	4:D:531:SER:HB2	2.14	0.47
1:T:118:DC:H2''	1:T:117:DG:OP2	2.13	0.47
4:D:707:ALA:HB1	4:D:771:ALA:HA	1.96	0.47
4:D:57:ARG:HD3	4:D:58:GLN:N	2.30	0.47
4:D:229:LEU:HD22	4:D:229:LEU:N	2.29	0.47
4:D:631:LYS:HE3	4:D:635:MET:CE	2.44	0.47
4:D:102:ALA:O	4:D:106:LEU:HD12	2.15	0.47
4:D:567:VAL:HB	4:D:880:PHE:CG	2.50	0.47
4:D:421:ASP:CG	4:D:423:ARG:NH1	2.73	0.46
4:D:485:ASN:O	4:D:486:HIS:C	2.57	0.46
4:D:689:VAL:CG1	4:D:692:ALA:HB3	2.43	0.46
2:N:20:DT:O4	4:D:168:GLU:OE1	2.33	0.46
3:R:2:A:H2'	5:R:901:APC:O4'	2.15	0.46
4:D:452:ILE:HG23	4:D:453:GLY:H	1.79	0.46
4:D:491:ALA:HB1	4:D:499:ASN:OD1	2.15	0.46
4:D:696:MET:HE3	4:D:697:ASN:HD21	1.80	0.46
1:T:111:DT:OP2	1:T:111:DT:H3'	2.15	0.46
4:D:109:ILE:HD12	4:D:109:ILE:N	2.30	0.46
4:D:203:SER:C	4:D:205:HIS:H	2.23	0.46
4:D:537:ASP:O	4:D:882:PHE:HD1	1.98	0.46
1:T:117:DG:H5''	4:D:421:ASP:CB	2.46	0.46
2:N:28:DG:H2''	2:N:29:DG:C8	2.50	0.46
4:D:126:LEU:HD11	4:D:244:ILE:HG22	1.96	0.46
4:D:298:ARG:HG3	4:D:420:MET:O	2.15	0.46
4:D:353:PRO:HD2	4:D:398:LEU:HD12	1.98	0.46
4:D:416:PHE:CE1	4:D:433:ASN:HA	2.50	0.46
4:D:150:ARG:O	4:D:150:ARG:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:588:ASN:O	4:D:613:THR:HG21	2.15	0.46
4:D:656:GLN:N	4:D:657:PRO:HD2	2.31	0.46
4:D:779:ALA:HB3	4:D:780:PRO:CD	2.45	0.46
4:D:57:ARG:HD3	4:D:58:GLN:HG3	1.96	0.46
4:D:54:MET:C	4:D:56:GLU:N	2.74	0.46
4:D:307:ARG:HG2	4:D:736:TRP:CH2	2.51	0.46
4:D:150:ARG:HA	4:D:150:ARG:HE	1.81	0.46
4:D:109:ILE:HG13	4:D:149:ALA:HA	1.97	0.46
2:N:29:DG:H2''	2:N:30:DC:OP2	2.15	0.46
4:D:248:PRO:O	4:D:252:GLU:CG	2.64	0.46
4:D:258:ALA:O	4:D:259:GLY:C	2.56	0.46
2:N:19:DG:C1'	2:N:20:DT:H73	2.42	0.45
4:D:248:PRO:O	4:D:252:GLU:CD	2.58	0.45
4:D:421:ASP:CG	4:D:423:ARG:HH12	2.24	0.45
4:D:576:LYS:NZ	4:D:576:LYS:CA	2.79	0.45
4:D:375:THR:O	4:D:375:THR:OG1	2.33	0.45
4:D:655:ILE:HG21	4:D:670:PRO:CB	2.46	0.45
1:T:130:DG:H8	1:T:130:DG:P	2.40	0.45
4:D:34:ARG:HH11	4:D:34:ARG:HG2	1.81	0.45
4:D:353:PRO:O	4:D:395:ARG:NH1	2.48	0.45
4:D:667:PHE:O	4:D:668:THR:C	2.59	0.45
4:D:744:GLN:HE21	4:D:758:GLN:HA	1.81	0.45
4:D:40:GLU:OE1	4:D:287:TRP:N	2.48	0.45
4:D:137:VAL:O	4:D:140:ALA:HB3	2.16	0.45
4:D:162:PHE:O	4:D:167:GLU:N	2.48	0.45
4:D:421:ASP:O	4:D:422:TRP:CD1	2.68	0.45
4:D:507:SER:O	4:D:511:PHE:HB2	2.17	0.45
4:D:832:MET:HE2	4:D:883:ALA:OXT	2.15	0.45
4:D:861:MET:CE	4:D:862:PRO:HD2	2.39	0.45
5:R:901:APC:H1'	4:D:784:HIS:HE1	1.80	0.45
4:D:210:ILE:HG13	4:D:211:HIS:N	2.31	0.45
4:D:89:PHE:O	4:D:92:VAL:N	2.50	0.45
2:N:17:DA:OP1	4:D:378:LYS:HD3	2.11	0.45
3:R:6:G:OP1	4:D:172:LYS:NZ	2.50	0.45
4:D:213:GLY:O	4:D:217:ILE:N	2.42	0.45
4:D:496:PRO:HG2	4:D:497:LEU:HG	1.99	0.45
4:D:741:LYS:O	4:D:742:PRO:C	2.60	0.45
4:D:210:ILE:HG13	4:D:211:HIS:H	1.82	0.44
4:D:671:ASN:O	4:D:672:GLN:HB3	2.17	0.44
1:T:127:DG:H2''	1:T:126:DT:C5	2.52	0.44
4:D:88:TRP:HB2	4:D:219:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:625:VAL:HG21	4:D:677:MET:CE	2.47	0.44
4:D:852:GLN:CD	4:D:853:LEU:N	2.75	0.44
4:D:446:LEU:HD13	4:D:806:SER:HB3	1.98	0.44
4:D:450:LYS:O	4:D:451:PRO:C	2.60	0.44
4:D:502:TRP:CZ3	4:D:512:LEU:HD22	2.52	0.44
4:D:46:MET:CE	4:D:269:GLN:NE2	2.80	0.44
4:D:61:ALA:O	4:D:62:GLY:C	2.61	0.44
4:D:705:LEU:HD13	4:D:854:HIS:HE1	1.82	0.44
4:D:756:ARG:N	4:D:756:ARG:NE	2.54	0.44
4:D:778:ILE:HG23	4:D:779:ALA:N	2.32	0.44
4:D:625:VAL:HG21	4:D:677:MET:HE1	1.98	0.44
4:D:782:PHE:O	4:D:786:GLN:HG2	2.17	0.44
4:D:90:GLU:O	4:D:93:LYS:HB2	2.18	0.44
4:D:118:THR:O	4:D:119:ILE:C	2.61	0.44
4:D:629:VAL:C	4:D:631:LYS:N	2.76	0.44
4:D:737:GLN:HE22	4:D:778:ILE:N	2.15	0.44
4:D:96:ARG:NE	4:D:96:ARG:HA	2.31	0.44
4:D:50:ARG:HG2	4:D:50:ARG:NH1	2.33	0.44
4:D:184:GLN:HA	4:D:184:GLN:NE2	2.33	0.44
4:D:104:GLN:HE21	4:D:104:GLN:CA	2.26	0.43
4:D:104:GLN:NE2	4:D:104:GLN:CA	2.79	0.43
4:D:463:HIS:CB	4:D:534:LEU:HD22	2.47	0.43
4:D:631:LYS:CD	4:D:632:ARG:N	2.77	0.43
4:D:720:ARG:HD2	4:D:721:LYS:N	2.34	0.43
1:T:124:DC:H1'	1:T:123:DG:C5'	2.48	0.43
1:T:116:DC:O5'	1:T:116:DC:H2'	2.19	0.43
4:D:126:LEU:HD21	4:D:244:ILE:O	2.18	0.43
4:D:135:GLN:HE21	4:D:241:SER:HA	1.83	0.43
4:D:172:LYS:HB3	4:D:173:ARG:NH2	2.33	0.43
1:T:119:DT:H5''	4:D:780:PRO:HG3	2.00	0.43
3:R:5:G:O2'	3:R:4:C:H5'	2.18	0.43
4:D:59:LEU:HD12	4:D:64:VAL:HG22	1.99	0.43
4:D:120:LYS:HE2	4:D:752:LEU:CD2	2.42	0.43
4:D:644:PHE:HE1	4:D:647:ARG:NH1	2.16	0.43
1:T:126:DT:H2''	1:T:125:DG:H5'	2.00	0.43
1:T:124:DC:H2''	1:T:123:DG:OP2	2.19	0.43
1:T:113:DT:H2''	1:T:112:DG:H5'	1.99	0.43
4:D:57:ARG:HD3	4:D:57:ARG:C	2.43	0.43
4:D:154:ILE:HA	4:D:159:ALA:HB3	2.01	0.43
4:D:201:TRP:HZ2	4:D:204:TRP:HE1	1.66	0.43
4:D:15:GLU:H	4:D:15:GLU:CD	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:24:LEU:HD21	4:D:287:TRP:CD2	2.54	0.43
4:D:402:LEU:HD12	4:D:402:LEU:HA	1.83	0.43
4:D:475:PHE:HB2	4:D:476:PRO:HD3	2.01	0.43
4:D:650:VAL:HG13	4:D:651:LEU:N	2.33	0.43
4:D:752:LEU:HD12	4:D:752:LEU:N	2.33	0.43
4:D:814:PHE:CD1	4:D:814:PHE:N	2.87	0.43
4:D:775:GLU:O	4:D:778:ILE:HG22	2.19	0.43
4:D:204:TRP:HZ3	4:D:212:VAL:HG11	1.84	0.43
4:D:217:ILE:O	4:D:221:ILE:HG13	2.19	0.42
4:D:714:LYS:C	4:D:715:THR:HG22	2.43	0.42
4:D:155:ARG:HH21	4:D:750:MET:HG2	1.84	0.42
4:D:386:ARG:HD3	4:D:387:LYS:H	1.80	0.42
4:D:500:THR:HA	4:D:502:TRP:NE1	2.34	0.42
4:D:698:TRP:CZ3	4:D:845:PHE:HD2	2.35	0.42
4:D:25:ALA:C	4:D:27:HIS:N	2.77	0.42
4:D:30:GLU:O	4:D:34:ARG:HG3	2.19	0.42
4:D:59:LEU:C	4:D:61:ALA:H	2.27	0.42
4:D:149:ALA:HB2	4:D:204:TRP:CZ2	2.54	0.42
4:D:320:ILE:HD11	4:D:426:VAL:HG22	2.00	0.42
4:D:631:LYS:CG	4:D:632:ARG:N	2.82	0.42
2:N:19:DG:N2	4:D:670:PRO:HD2	2.35	0.42
4:D:160:LYS:C	4:D:162:PHE:N	2.77	0.42
4:D:296:LEU:HD22	4:D:317:TYR:CE1	2.55	0.42
4:D:402:LEU:HD13	4:D:439:MET:CE	2.49	0.42
4:D:502:TRP:CD2	4:D:512:LEU:HD13	2.54	0.42
4:D:810:ILE:O	4:D:810:ILE:HG22	2.19	0.42
4:D:791:LEU:HD12	4:D:811:HIS:O	2.20	0.42
4:D:162:PHE:CD1	4:D:167:GLU:HB2	2.55	0.42
4:D:828:VAL:HG13	4:D:882:PHE:O	2.20	0.42
4:D:132:THR:O	4:D:244:ILE:N	2.45	0.42
4:D:150:ARG:C	4:D:152:GLY:H	2.28	0.42
4:D:420:MET:HA	4:D:425:ARG:O	2.20	0.42
4:D:631:LYS:C	4:D:631:LYS:CD	2.88	0.42
4:D:685:VAL:HG13	4:D:686:SER:N	2.34	0.42
1:T:120:DT:C2'	1:T:119:DT:OP2	2.53	0.41
4:D:117:ILE:HG23	4:D:752:LEU:CD2	2.49	0.41
4:D:170:LEU:HD11	4:D:179:LYS:HB3	2.02	0.41
4:D:533:PRO:HA	4:D:816:THR:O	2.20	0.41
4:D:721:LYS:O	4:D:722:ARG:C	2.62	0.41
4:D:747:LEU:HD23	4:D:755:PHE:O	2.20	0.41
4:D:143:ARG:HG2	4:D:143:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:MET:H	4:D:222:GLU:CG	2.34	0.41
4:D:245:GLU:C	4:D:246:LEU:HD22	2.44	0.41
4:D:653:ASP:O	4:D:657:PRO:HG3	2.20	0.41
4:D:712:ASP:O	4:D:716:GLY:CA	2.67	0.41
4:D:852:GLN:NE2	4:D:852:GLN:C	2.78	0.41
2:N:20:DT:C2'	2:N:21:DT:H72	2.47	0.41
3:R:2:A:C2'	5:R:901:APC:H5'1	2.50	0.41
4:D:183:MET:HE3	4:D:183:MET:O	2.19	0.41
1:T:120:DT:O5'	1:T:120:DT:H2'	2.20	0.41
4:D:40:GLU:OE2	4:D:286:TYR:HB3	2.20	0.41
4:D:506:ASP:OD2	4:D:506:ASP:N	2.43	0.41
4:D:799:HIS:HD2	4:D:804:ILE:O	2.03	0.41
4:D:843:ALA:O	4:D:847:ASP:OD2	2.38	0.41
4:D:853:LEU:H	4:D:853:LEU:CD1	2.30	0.41
4:D:151:PHE:O	4:D:153:ARG:N	2.43	0.41
4:D:424:GLY:O	4:D:792:ARG:NH1	2.54	0.41
4:D:655:ILE:C	4:D:657:PRO:HD2	2.46	0.41
4:D:749:LEU:O	4:D:750:MET:HB2	2.20	0.41
4:D:826:LYS:O	4:D:827:ALA:C	2.62	0.41
4:D:268:PHE:HB3	4:D:286:TYR:OH	2.21	0.41
4:D:576:LYS:HA	4:D:576:LYS:CE	2.50	0.41
4:D:860:LYS:O	4:D:862:PRO:HD3	2.20	0.41
1:T:115:DC:C4'	4:D:431:MET:HE3	2.51	0.41
4:D:272:VAL:HG12	4:D:411:HIS:CD2	2.55	0.41
4:D:297:VAL:CG1	4:D:422:TRP:HA	2.50	0.41
4:D:459:TRP:O	4:D:534:LEU:CD1	2.68	0.41
4:D:579:ASN:HA	4:D:579:ASN:HD22	1.70	0.41
4:D:19:ILE:HG23	4:D:19:ILE:O	2.20	0.41
4:D:165:ASN:C	4:D:169:GLN:HE22	2.29	0.41
4:D:357:ARG:HA	4:D:388:ASP:OD2	2.20	0.41
4:D:826:LYS:O	4:D:828:VAL:O	2.39	0.41
4:D:378:LYS:HE2	4:D:378:LYS:HB3	1.84	0.41
4:D:789:SER:O	4:D:793:LYS:HB2	2.20	0.41
4:D:134:VAL:HG23	4:D:135:GLN:N	2.36	0.41
4:D:264:ILE:HG22	4:D:292:ARG:HG3	2.03	0.41
4:D:361:PRO:O	4:D:362:MET:CB	2.69	0.41
4:D:701:SER:O	4:D:705:LEU:HG	2.21	0.41
1:T:126:DT:H2''	1:T:125:DG:OP2	2.21	0.40
4:D:275:PRO:HB2	4:D:324:GLN:HG3	2.01	0.40
4:D:357:ARG:HG2	4:D:357:ARG:NH1	2.36	0.40
4:D:151:PHE:C	4:D:151:PHE:CD1	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:311:VAL:CG2	4:D:313:MET:SD	3.09	0.40
4:D:349:VAL:O	4:D:351:ASP:N	2.54	0.40
4:D:551:ARG:HG3	4:D:551:ARG:HH11	1.85	0.40
4:D:659:ILE:O	4:D:661:SER:N	2.54	0.40
4:D:671:ASN:C	4:D:673:ALA:N	2.79	0.40
4:D:274:PRO:HA	4:D:275:PRO:HD3	1.96	0.40
4:D:308:TYR:O	4:D:309:GLU:C	2.64	0.40
4:D:328:TRP:CH2	4:D:434:PRO:HB3	2.56	0.40
4:D:544:GLN:HA	4:D:559:VAL:HG21	2.03	0.40
4:D:644:PHE:HE1	4:D:647:ARG:CZ	2.34	0.40
4:D:33:ALA:O	4:D:37:LEU:HD22	2.22	0.40
4:D:297:VAL:HG13	4:D:422:TRP:HA	2.03	0.40
4:D:337:VAL:HG21	4:D:512:LEU:HD21	2.03	0.40
4:D:637:LEU:HD22	4:D:685:VAL:HG13	2.02	0.40
4:D:42:GLU:CG	4:D:46:MET:HE2	2.48	0.40
4:D:330:ILE:HD12	4:D:405:ALA:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	821/883 (93%)	663 (81%)	111 (14%)	47 (6%)	1 4

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	15	GLU
4	D	149	ALA
4	D	226	MET
4	D	360	LEU
4	D	422	TRP

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Mol	Chain	Res	Type
4	D	460	LEU
4	D	613	THR
4	D	614	LYS
4	D	716	GLY
4	D	764	ASN
4	D	767	SER
4	D	829	ARG
4	D	857	GLN
4	D	16	LEU
4	D	20	PRO
4	D	437	ASN
4	D	501	TRP
4	D	586	ALA
4	D	661	SER
4	D	762	ASN
4	D	854	HIS
4	D	859	ASP
4	D	192	SER
4	D	205	HIS
4	D	230	HIS
4	D	350	GLU
4	D	351	ASP
4	D	357	ARG
4	D	500	THR
4	D	630	THR
4	D	668	THR
4	D	850	ALA
4	D	853	LEU
4	D	148	GLU
4	D	157	LEU
4	D	164	LYS
4	D	200	ALA
4	D	344	TRP
4	D	659	ILE
4	D	669	GLN
4	D	882	PHE
4	D	118	THR
4	D	260	ALA
4	D	660	ASP
4	D	114	VAL
4	D	434	PRO
4	D	559	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	
4	D	683/729 (94%)	637 (93%)	46 (7%)	15	39

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	27	HIS
4	D	37	LEU
4	D	50	ARG
4	D	109	ILE
4	D	120	LYS
4	D	126	LEU
4	D	154	ILE
4	D	169	GLN
4	D	232	GLN
4	D	257	ARG
4	D	281	ILE
4	D	311	VAL
4	D	313	MET
4	D	318	LYS
4	D	325	ASN
4	D	335	LEU
4	D	350	GLU
4	D	362	MET
4	D	377	TRP
4	D	402	LEU
4	D	419	ASN
4	D	423	ARG
4	D	443	LEU
4	D	472	LYS
4	D	506	ASP
4	D	514	PHE
4	D	565	GLU
4	D	567	VAL
4	D	576	LYS
4	D	577	LYS

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Mol	Chain	Res	Type
4	D	587	ILE
4	D	588	ASN
4	D	631	LYS
4	D	665	LEU
4	D	666	MET
4	D	683	GLU
4	D	715	THR
4	D	743	ILE
4	D	747	LEU
4	D	756	ARG
4	D	793	LYS
4	D	816	THR
4	D	831	THR
4	D	852	GLN
4	D	855	GLU
4	D	859	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
4	D	22	ASN
4	D	67	ASN
4	D	86	ASN
4	D	104	GLN
4	D	131	ASN
4	D	135	GLN
4	D	165	ASN
4	D	169	GLN
4	D	184	GLN
4	D	211	HIS
4	D	232	GLN
4	D	321	ASN
4	D	339	ASN
4	D	404	GLN
4	D	406	ASN
4	D	419	ASN
4	D	433	ASN
4	D	435	GLN
4	D	466	ASN
4	D	485	ASN
4	D	488	ASN
4	D	505	GLN

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Mol	Chain	Res	Type
4	D	568	GLN
4	D	579	ASN
4	D	648	GLN
4	D	649	GLN
4	D	669	GLN
4	D	697	ASN
4	D	726	HIS
4	D	737	GLN
4	D	744	GLN
4	D	762	ASN
4	D	764	ASN
4	D	781	ASN
4	D	784	HIS
4	D	786	GLN
4	D	799	HIS
4	D	854	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	R	8/9 (88%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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
5	APC	R	901	6	29,33,33	1.35	3 (10%)	44,52,52	1.85	7 (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
5	APC	R	901	6	-	3/19/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	901	APC	PB-O3B	3.94	1.62	1.58
5	R	901	APC	PA-O2A	-3.12	1.48	1.56
5	R	901	APC	PB-O2B	-3.10	1.48	1.56

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	901	APC	C1'-N9-C8	-6.27	113.17	127.09
5	R	901	APC	C4-N9-C1'	5.81	140.21	126.63
5	R	901	APC	O1B-PB-C3A	-5.07	95.69	109.05
5	R	901	APC	O2A-PA-O1A	3.02	119.78	109.95
5	R	901	APC	O2B-PB-O1B	2.86	119.25	109.95
5	R	901	APC	O2B-PB-C3A	2.28	116.16	106.73
5	R	901	APC	O2G-PG-O1G	2.24	119.57	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

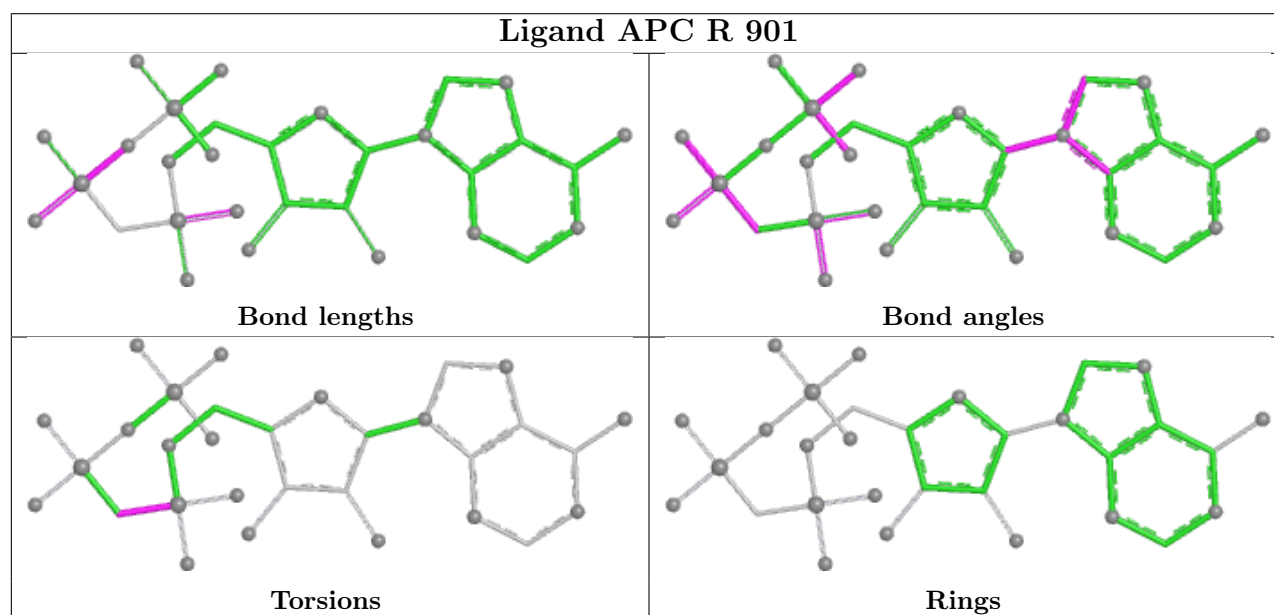
Mol	Chain	Res	Type	Atoms
5	R	901	APC	PB-C3A-PA-O1A
5	R	901	APC	PB-C3A-PA-O5'
5	R	901	APC	PB-C3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	901	APC	11	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 [i](#)

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

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	T	21/21 (100%)	-1.78	0 100 100	43, 97, 136, 138	0
2	N	17/17 (100%)	-1.55	0 100 100	121, 128, 138, 142	0
3	R	9/9 (100%)	-1.62	0 100 100	72, 96, 103, 104	0
4	D	829/883 (93%)	-1.66	0 100 100	0, 26, 74, 97	0
All	All	876/930 (94%)	-1.66	0 100 100	0, 29, 93, 142	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

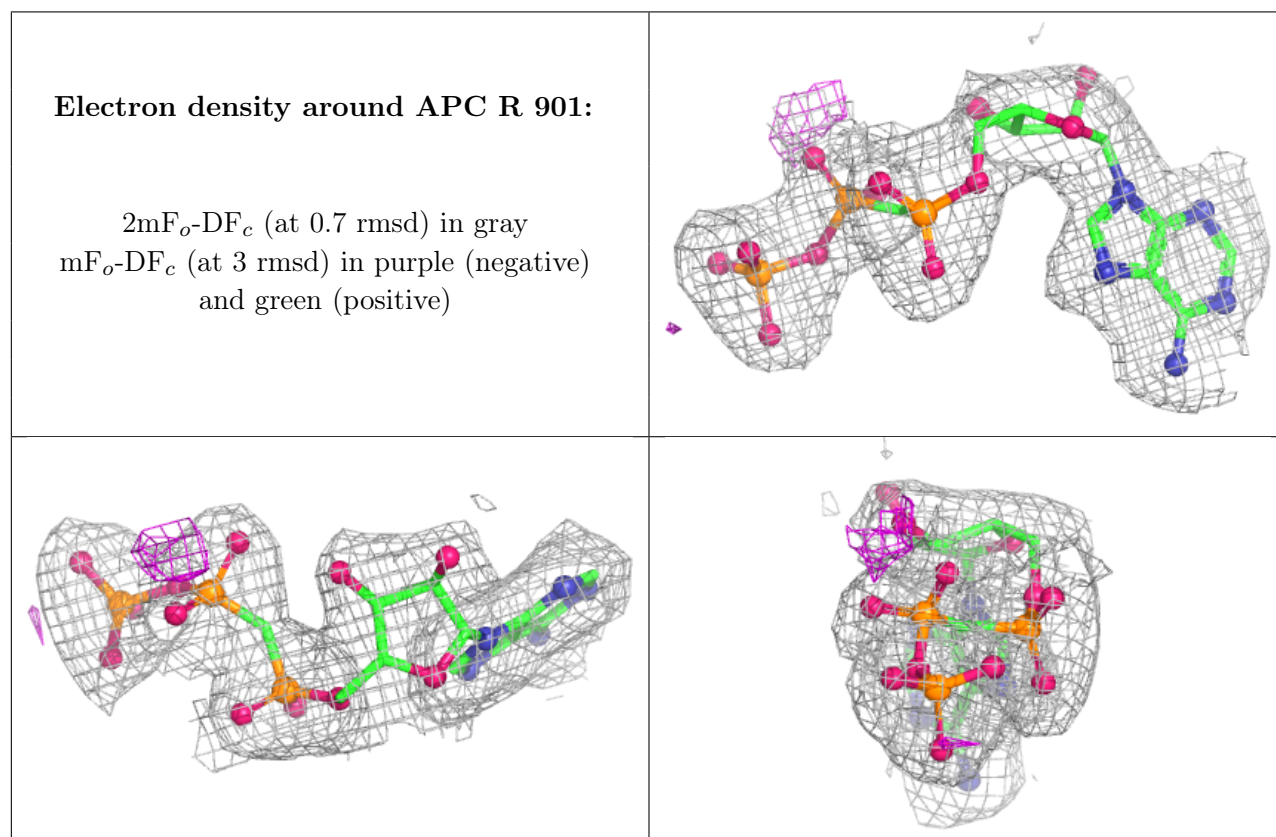
There are no oligosaccharides in this entry.

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	MG	D	902	1/1	0.99	0.02	23,23,23,23	0
6	MG	D	903	1/1	0.99	0.05	31,31,31,31	0
5	APC	R	901	31/31	1.00	0.02	13,23,44,67	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.