



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 08:30 pm BST

PDB ID : 1S76
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

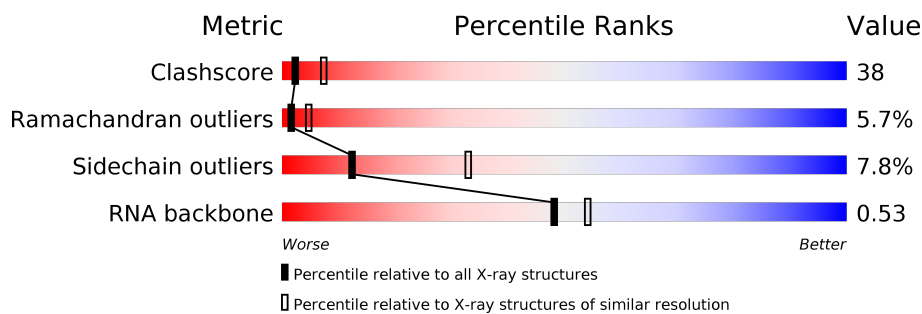
1 Overall quality at a glance

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	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RNA backbone	3102	1121 (3.16-2.60)

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 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 $\leq 5\%$.

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			

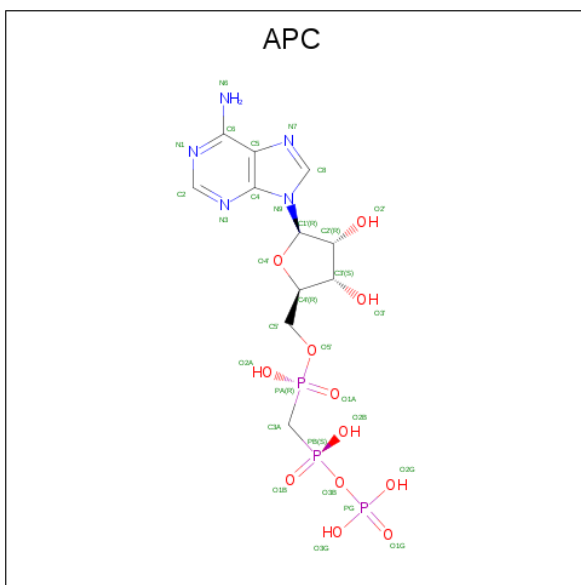
- Molecule 3 is a RNA chain called RNA (5'-R(P*AP*CP*AP*CP*GP*GP*CP*GP*A)-3').

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 (three-letter code: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).



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

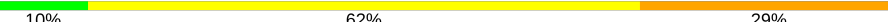
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

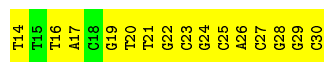
- Molecule 1: DNA (5'-D(P*GP*CP*CP*GP*TP*GP*CP*GP*CP*AP*TP*TP*CP*GP*CP*C P*GP*TP*GP*TP*T)-3')

Chain T: 



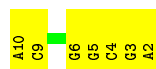
- Molecule 2: DNA (5'-D(P*TP*TP*TP*AP*CP*GP*TP*TP*GP*CP*GP*CP*AP*CP*GP*G P*C)-3')

Chain N: 



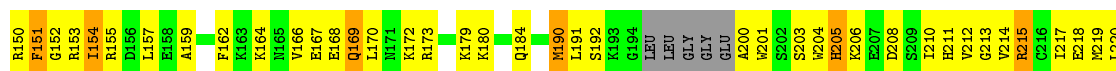
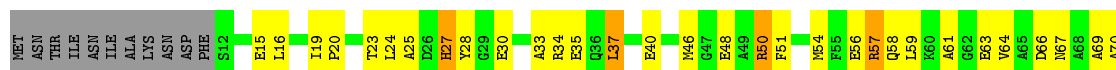
- Molecule 3: RNA (5'-R(P*AP*CP*AP*CP*GP*GP*CP*GP*A)-3')

Chain R: 



- Molecule 4: DNA-directed RNA polymerase

Chain D: 



B811	R746	A674	SER	G538	K450	W287
D812	L747	G675	GLU	S539	P451	A288
S813	N748	G676	LYS	C540	I452	
F814	L749	M677	VAL		G453	R292
G815	M750		LYS	I543		
T816	F751	L680	LEU	Q544	Q456	L296
P818	L752	I681		F545		V297
		W682	T613	F546	W459	R298
L824	R755	E683	K614	S547	L460	
P825	F756	S684	A615		K461	K303
K826	L757	V685	L616	L550	I462	
	Q758	S686		R551	H463	R307
A827	P759		W625	D552		Y308
R828	T760	V689	T626	E553	M466	E309
R829	I761	N762	R627	V554	C467	D310
E830	N762	A692	S628		A468	V311
T831	T763		V629	R557		Y312
	M764	A695	T630	A558	K472	M313
A843	K765		K631	V559	V473	
D844	D766	W698	B632	M560	P474	L398
F845	S767		S633	L561	F475	E399
Y846	E768	S701	V634		P476	F400
D847	I769		B635	S564	E477	M401
Q848	D770	K704	T636	E565	R478	N321
F849	T771	L705	L637	T566	I479	Q324
A850		L706	A638	V567		N325
D851	E775	A707	V639		M485	
		A708	G640	Y571	H486	W328
Q852	L778	E709	S641		E487	K329
B853	A779	D712		V574	M488	I330
E855	N780		F644	A575		
S856	N781	T715	G645	K576	A491	L335
Q857	F782	G716	F646	K577	C492	A336
L858	R783		B647	V578		V337
D859	H784		Q648	N579	S495	A338
K860	S785	R720	Q649	E580	P496	N339
N861	Q786	K721	Q650	I581	L497	
P862	R722	L781	L651	L582	M420	K343
G788	G783	G723	B652	Q583	N499	
S789	D783	A724	D653	A584	W422	
H790	V725	V725	W654	D585	R423	
L791	H726		I655	A586	T500	W344
R792			Q656	I587	W501	V349
K793	T729	T729	P657	N588	W502	E350
	F730	P730	A658	Q505	A503	D351
V795	D731	L731	L659	E589	E504	I352
V796	G732	G732	D660	T590	D506	P353
F797	F733	F733	S661		S507	A354
A798	T734	T734	G662	VAL	P508	I355
H799	H735	H735	K663	THR		E356
E800	W736	W736	G664	L512	F511	E359
K801	L601	L601	L665	VAL	A513	L360
Y802	Q737	Q737	W666	THR	F514	P361
	E738	E738	F667	ASP		M361
G803	V739	V739		GLU		W362
I804	K740	K740	T668	LYS	M439	
E805	E741	E741	Q669	ASN	M433	LYS
S806	F742	F742	P670	THR	Q435	PRO
	I743	I743	N671	GLY	L443	GLU
L809	Q744	Q744	Q672	GLU	L446	ASP
I810	T745	T745	A672	ILE		ILE

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 29.53 – 2.88	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.88) 91.2 (29.53-2.88)	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 0.211 , (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)	0.06 , 458.1	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	0.90	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	0.57	1/478 (0.2%)	0.85	0/734
2	N	0.50	1/388 (0.3%)	0.69	0/595
3	R	0.72	1/219 (0.5%)	0.83	0/338
4	D	0.36	2/6706 (0.0%)	0.58	1/9068 (0.0%)
All	All	0.40	5/7791 (0.1%)	0.62	1/10735 (0.0%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	14	DT	OP3-P	-7.30	1.52	1.61
3	R	10	A	OP3-P	-7.28	1.52	1.61
1	T	130	DG	OP3-P	-7.24	1.52	1.61
4	D	292	ARG	C-N	-6.38	1.22	1.34
4	D	251	ALA	C-N	5.80	1.47	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	828	VAL	N-CA-C	-5.01	97.48	111.00

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
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	28	0
2	N	348	0	193	26	0
3	R	196	0	100	15	0
4	D	6555	0	6518	509	0
5	R	31	0	14	11	0
6	D	2	0	0	0	0
All	All	7561	0	7063	561	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 38.

All (561) 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:724:ALA:HB2	4:D:738:GLU:HB3	1.36	1.06
4:D:763:THR:O	4:D:764:ASN:CG	1.96	1.04
3:R:2:A:O3'	5:R:901:APC:C5'	2.09	1.01
4:D:861:MET:HE3	4:D:862:PRO:HD2	1.44	1.00
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:D:756:ARG:HE	4:D:756:ARG:H	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
4:D:756:ARG:N	4:D:756:ARG:HE	1.74	0.85
1:T:120:DT:H2''	1:T:119:DT:OP2	1.76	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
4:D:358:GLU:OE1	4:D:387:LYS:HD2	1.81	0.81
2:N:17:DA:P	4:D:378:LYS:HD3	2.19	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:386:ARG:HD3	4:D:387:LYS:N	1.97	0.79
4:D:873:ARG:HH11	4:D:873:ARG:HG3	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: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
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)
3:R:2:A:H2'	5:R:901:APC:H8	1.67	0.75
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: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:864:LEU:HD12	4:D:864:LEU:H	1.56	0.69
4:D:154:ILE:H	4:D:154:ILE:HD12	1.56	0.69
3:R:2:A:O2'	5:R:901:APC:O4'	2.10	0.69
4:D:806:SER:O	4:D:816:THR:HG23	1.92	0.69
4:D:756:ARG:H	4:D:756:ARG:NE	1.91	0.69
4:D:565:GLU:OE2	4:D:566:THR:HG22	1.93	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:466:ASN:HD21	4:D:478:ARG:HH11	1.40	0.68
4:D:85:ILE:HA	4:D:219:MET:HE2	1.76	0.68
4:D:126:LEU:HA	4:D:132:THR:CG2	2.24	0.68
4:D:360:LEU:N	4:D:361:PRO:HD2	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:298:ARG:HE	4:D:419:ASN:ND2	1.91	0.68
4:D:85:ILE:HA	4:D:219:MET:CE	2.23	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:853:LEU:H	4:D:853:LEU:HD12	1.60	0.67
4:D:829:ARG:NH2	4:D:882:PHE:H	1.93	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:N	4:D:154:ILE:HD12	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
4:D:219:MET:HA	4:D:222:GLU:HB2	1.77	0.66
2:N:27:DC:H2''	2:N:28:DG:C5'	2.25	0.66
4:D:88:TRP:CZ2	4:D:215:ARG:HD3	2.31	0.66
4:D:423:ARG:HB2	4:D:423:ARG:NH1	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: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: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: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:767:SER:O	4:D:768:GLU:HB3	1.98	0.63
4:D:419:ASN:C	4:D:419:ASN:HD22	2.01	0.63
4:D:639:TYR:HE1	4:D:783:VAL:HG21	1.63	0.63
4:D:631:LYS:C	4:D:631:LYS:HD2	2.20	0.62
4:D:854:HIS:O	4:D:858:LEU:HB2	1.99	0.62
4:D:104:GLN:HE21	4:D:104:GLN:HA	1.63	0.62
1:T:124:DC:H1'	1:T:123:DG:H5'	1.80	0.62
4:D:46:MET:HE1	4:D:269:GLN:NE2	2.15	0.62
3:R:2:A:C3'	5:R:901:APC:H5'1	2.28	0.62
4:D:204:TRP:O	4:D:208:ASP:HB2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:473:VAL:HG21	4:D:477:GLU:OE1	2.00	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:362:MET:C	4:D:381:ALA:HB2	2.22	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:298:ARG:NH2	4:D:419:ASN:HD21	1.98	0.60
4:D:286:TYR:CZ	4:D:417:PRO:HG3	2.37	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:378:LYS:C	4:D:378:LYS:HD2	2.22	0.59
4:D:40:GLU:CD	4:D:286:TYR:HB3	2.22	0.59
4:D:71:LYS:N	4:D:72:PRO:HD2	2.17	0.59
4:D:747:LEU:N	4:D:747:LEU:HD23	2.18	0.59
4:D:576:LYS:HA	4:D:576:LYS:NZ	2.17	0.59
4:D:118:THR:O	4:D:122:THR:HG23	2.03	0.59
4:D:151:PHE:C	4:D:153:ARG:H	2.06	0.59
4:D:169:GLN:NE2	4:D:169:GLN:H	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:663:LYS:CD	4:D:663:LYS:H	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:402:LEU:HD13	4:D:439:MET:HE3	1.84	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
4:D:88:TRP:O	4:D:92:VAL:HG23	2.04	0.58
4:D:551:ARG:O	4:D:870:LEU:HB3	2.04	0.57
1:T:120:DT:H5'	4:D:641:SER:HA	1.86	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:143:ARG:HH21	4:D:206:LYS:HG2	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:544:GLN:HG2	4:D:559:VAL:HB	1.86	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: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
2:N:28:DG:H2"	2:N:29:DG:N7	2.19	0.57
4:D:218:GLU:C	4:D:220:LEU:H	2.07	0.57
4:D:759:PRO:HG2	4:D:764:ASN:HD22	1.61	0.57
4:D:125:CYS:HA	4:D:128:SER:OG	2.04	0.57
2:N:17:DA:OP1	4:D:378:LYS:CD	2.53	0.57
4:D:115:ALA:O	4:D:118:THR:HB	2.04	0.57
2:N:27:DC:C1'	2:N:28:DG:H5"	2.30	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:228:SER:HB2	4:D:245:GLU:CG	2.36	0.56
4:D:226:MET:HA	4:D:250:TYR:HD1	1.71	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:473:VAL:HG21	4:D:477:GLU:CD	2.25	0.56
4:D:629:VAL:O	4:D:631:LYS:N	2.36	0.56
4:D:613:THR:HG23	4:D:676:TYR:CE1	2.41	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
4:D:816:THR:OG1	4:D:824:LEU:HD22	2.05	0.55
4:D:473:VAL:HG22	4:D:474:PRO:CD	2.34	0.55
4:D:61:ALA:O	4:D:63:GLU:HG3	2.07	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:HD12	4:D:752:LEU:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:472:LYS:NZ	4:D:472:LYS:HB2	2.21	0.55
4:D:70:ALA:C	4:D:72:PRO:HD2	2.26	0.55
4:D:143:ARG:NH2	4:D:206:LYS:HG2	2.22	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
1:T:115:DC:H2"	1:T:114:DG:H5'	1.88	0.55
2:N:22:DG:H2"	2:N:23:DC:C5	2.41	0.54
1:T:120:DT:C4	4:D:636:THR:HG21	2.41	0.54
4:D:48:GLU:HG2	4:D:262:ALA:C	2.26	0.54
4:D:565:GLU:CG	4:D:566:THR:N	2.69	0.54
4:D:500:THR:O	4:D:501:TRP:CB	2.55	0.54
1:T:119:DT:H2"	1:T:118:DC:OP2	2.07	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: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
4:D:579:ASN:HD22	4:D:582:LEU:HD12	1.72	0.54
4:D:629:VAL:C	4:D:631:LYS:H	2.11	0.54
2:N:27:DC:H2"	2:N:28:DG:O5'	2.08	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
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
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
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: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
4:D:25:ALA:C	4:D:27:HIS:H	2.11	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:2:A:H2'	5:R:901:APC:C8	2.35	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:N	4:D:746:ARG:HD3	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:810:ILE:O	4:D:811:HIS:HB2	2.09	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:576:LYS:HZ1	4:D:576:LYS:HA	1.74	0.53
4:D:416:PHE:CE2	4:D:434:PRO:HD3	2.43	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
2:N:27:DC:H1'	2:N:28:DG:OP1	2.08	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:HD12	4:D:264:ILE:O	2.08	0.52
4:D:421:ASP:OD1	4:D:423:ARG:NH1	2.37	0.52
4:D:104:GLN:NE2	4:D:104:GLN:HA	2.24	0.52
4:D:881:ALA:O	4:D:882:PHE:HB2	2.09	0.52
4:D:538:GLY:HA3	4:D:883:ALA:HB3	1.91	0.52
4:D:743:ILE:CD1	4:D:744:GLN:H	2.23	0.52
4:D:704:LYS:HB2	4:D:775:GLU:OE2	2.09	0.52
4:D:152:GLY:CA	4:D:155:ARG:HD3	2.38	0.52
4:D:550:LEU:HD11	4:D:695:ALA:CB	2.38	0.52
4:D:155:ARG:CD	4:D:155:ARG:H	2.23	0.52
4:D:85:ILE:HD13	4:D:219:MET:SD	2.49	0.52
4:D:141:ILE:O	4:D:145:ILE:HG12	2.10	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:421:ASP:O	4:D:422:TRP:CB	2.58	0.51
4:D:856:SER:O	4:D:857:GLN:CB	2.53	0.51
4:D:85:ILE:HD13	4:D:219:MET:CE	2.41	0.51
4:D:24:LEU:O	4:D:28:TYR:N	2.39	0.51
4:D:731:ASP:OD2	4:D:792:ARG:NE	2.43	0.51
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:308:TYR:HE2	4:D:734:PRO:HG2	1.75	0.50
4:D:343:LYS:HA	4:D:355:ILE:HD11	1.94	0.50
4:D:67:ASN:ND2	4:D:69:ALA:H	2.03	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
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:419:ASN:C	4:D:419:ASN:ND2	2.64	0.50
4:D:547:SER:HA	4:D:552:ASP:HB3	1.94	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:303:LYS:H	4:D:303:LYS:HE2	1.77	0.50
4:D:35:GLU:HG2	4:D:272:VAL:HG21	1.92	0.50
4:D:655:ILE:O	4:D:659:ILE:HG12	2.12	0.50
4:D:307:ARG:HG2	4:D:736:TRP:CE3	2.47	0.50
4:D:852:GLN:O	4:D:853:LEU:C	2.50	0.50
4:D:308:TYR:HA	4:D:311:VAL:CG1	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:855:GLU:CD	4:D:856:SER:H	2.14	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:766:ASP:O	4:D:767:SER:CB	2.57	0.49
4:D:146:GLU:C	4:D:148:GLU:H	2.14	0.49
4:D:85:ILE:HA	4:D:219:MET:HE1	1.94	0.49
4:D:378:LYS:HD2	4:D:378:LYS:O	2.13	0.49
4:D:357:ARG:HG2	4:D:357:ARG:HH11	1.77	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:57:ARG:HG2	4:D:57:ARG:HH11	1.78	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
4:D:353:PRO:HD2	4:D:398:LEU:CD1	2.43	0.49
3:R:2:A:C2'	5:R:901:APC:O4'	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:724:ALA:HB2	4:D:738:GLU:CB	2.25	0.49
1:T:122:DC:H2"	1:T:121:DA:OP2	2.12	0.49
4:D:565:GLU:HG2	4:D:566:THR:H	1.75	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
4:D:645:GLY:O	4:D:649:GLN:HG3	2.14	0.48
1:T:130:DG:H2"	1:T:129:DC:H5	1.78	0.48
4:D:228:SER:C	4:D:229:LEU:HD22	2.34	0.48
4:D:423:ARG:HH21	4:D:784:HIS:CD2	2.31	0.48
4:D:66:ASP:O	4:D:71:LYS:NZ	2.44	0.48
2:N:22:DG:H2"	2:N:23:DC:H5	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
3:R:9:C:H5'	4:D:746:ARG:HH22	1.78	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: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
4:D:613:THR:O	4:D:614:LYS:C	2.52	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
1:T:126:DT:H1'	1:T:125:DG:H5"	1.96	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:CD1	4:D:109:ILE:H	2.25	0.47
4:D:298:ARG:HE	4:D:419:ASN:CG	2.18	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
4:D:707:ALA:HB1	4:D:771:ALA:HA	1.96	0.47
1:T:118:DC:H2"	1:T:117:DG:OP2	2.13	0.47
4:D:229:LEU:HD22	4:D:229:LEU:N	2.29	0.47
4:D:57:ARG:HD3	4:D:58:GLN:N	2.30	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:671:ASN:C	4:D:673:ALA:H	2.18	0.47
4:D:567:VAL:HB	4:D:880:PHE:CG	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:R:2:A:H2'	5:R:901:APC:O4'	2.15	0.46
4:D:109:ILE:N	4:D:109:ILE:HD12	2.30	0.46
4:D:537:ASP:O	4:D:882:PHE:HD1	1.98	0.46
1:T:111:DT:H3'	1:T:111:DT:OP2	2.15	0.46
4:D:126:LEU:HD11	4:D:244:ILE:HG22	1.96	0.46
4:D:353:PRO:HD2	4:D:398:LEU:HD12	1.98	0.46
4:D:298:ARG:HG3	4:D:420:MET:O	2.15	0.46
4:D:416:PHE:CE1	4:D:433:ASN:HA	2.50	0.46
2:N:28:DG:H2''	2:N:29:DG:C8	2.50	0.46
1:T:117:DG:H5''	4:D:421:ASP:CB	2.46	0.46
4:D:104:GLN:CA	4:D:104:GLN:NE2	2.79	0.46
4:D:150:ARG:O	4:D:150:ARG:HG3	2.15	0.46
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:565:GLU:CD	4:D:566:THR:H	2.18	0.46
4:D:57:ARG:HD3	4:D:58:GLN:HG3	1.96	0.46
4:D:307:ARG:HG2	4:D:736:TRP:CH2	2.51	0.46
4:D:150:ARG:HE	4:D:150:ARG:HA	1.81	0.46
4:D:109:ILE:HG13	4:D:149:ALA:HA	1.97	0.46
4:D:248:PRO:O	4:D:252:GLU:CG	2.64	0.46
2:N:29:DG:H2''	2:N:30:DC:OP2	2.15	0.46
4:D:576:LYS:CA	4:D:576:LYS:NZ	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
4:D:34:ARG:HG2	4:D:34:ARG:HH11	1.81	0.45
4:D:353:PRO:O	4:D:395:ARG:NH1	2.48	0.45
4:D:398:LEU:HD23	4:D:398:LEU:C	2.36	0.45
1:T:130:DG:H8	1:T:130:DG:P	2.40	0.45
4:D:744:GLN:HE21	4:D:758:GLN:HA	1.81	0.45
4:D:861:MET:HE3	4:D:862:PRO:CD	2.30	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:40:GLU:OE1	4:D:287:TRP: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:210:ILE:HG13	4:D:211:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:901:APC:H1'	4:D:784:HIS:HE1	1.80	0.45
4:D:551:ARG:C	4:D:870:LEU:HB3	2.37	0.45
4:D:89:PHE:O	4:D:92:VAL:N	2.50	0.45
4:D:213:GLY:O	4:D:217:ILE:N	2.42	0.45
4:D:218:GLU:C	4:D:220:LEU:N	2.71	0.45
2:N:17:DA:OP1	4:D:378:LYS:HD3	2.11	0.45
4:D:496:PRO:HG2	4:D:497:LEU:HG	1.99	0.45
3:R:6:G:OP1	4:D:172:LYS:NZ	2.50	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
4:D:625:VAL:HG21	4:D:677:MET:CE	2.47	0.44
1:T:127:DG:H2"	1:T:126:DT:C5	2.52	0.44
4:D:502:TRP:CZ3	4:D:512:LEU:HD22	2.52	0.44
4:D:446:LEU:HD13	4:D:806:SER:HB3	1.98	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:737:GLN:HE22	4:D:778:ILE:N	2.15	0.44
4:D:855:GLU:CD	4:D:856:SER:N	2.71	0.44
4:D:90:GLU:O	4:D:93:LYS:HB2	2.18	0.44
4:D:763:THR:C	4:D:764:ASN:CG	2.74	0.44
4:D:96:ARG:HA	4:D:96:ARG:NE	2.31	0.44
4:D:184:GLN:NE2	4:D:184:GLN:HA	2.33	0.44
4:D:50:ARG:HG2	4:D:50:ARG:NH1	2.33	0.44
4:D:433:ASN:C	4:D:435:GLN:H	2.22	0.43
4:D:104:GLN:CA	4:D:104:GLN:HE21	2.26	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:116:DC:O5'	1:T:116:DC:H2'	2.19	0.43
1:T:124:DC:H1'	1:T:123:DG:C5'	2.48	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
4:D:126:LEU:HD21	4:D:244:ILE:O	2.18	0.43
4:D:120:LYS:HE2	4:D:752:LEU:CD2	2.42	0.43
4:D:88:TRP:HB2	4:D:219:MET:HE3	2.01	0.43
4:D:59:LEU:HD12	4:D:64:VAL:HG22	1.99	0.43
4:D:644:PHE:HE1	4:D:647:ARG:NH1	2.16	0.43
1:T:119:DT:H5"	4:D:780:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:5:G:O2'	3:R:4:C:H5'	2.18	0.43
4:D:151:PHE:C	4:D:153:ARG:N	2.71	0.43
1:T:126:DT:H2''	1:T:125:DG:H5'	2.00	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
1:T:113:DT:H2''	1:T:112:DG:H5'	1.99	0.43
1:T:124:DC:H2''	1:T:123:DG:OP2	2.19	0.43
4:D:24:LEU:HD21	4:D:287:TRP:CD2	2.54	0.43
4:D:402:LEU:HA	4:D:402:LEU:HD12	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:N	4:D:814:PHE:CD1	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:46:MET:CE	4:D:269:GLN:NE2	2.80	0.42
4:D:810:ILE:O	4:D:810:ILE:HG22	2.19	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:149:ALA:HB2	4:D:204:TRP:CZ2	2.54	0.42
4:D:30:GLU:O	4:D:34:ARG:HG3	2.19	0.42
4:D:190:MET:HE3	4:D:191:LEU:H	1.83	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
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
2:N:19:DG:N2	4:D:670:PRO:HD2	2.35	0.42
4:D:248:PRO:O	4:D:252:GLU:CD	2.58	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:421:ASP:CG	4:D:423:ARG:NH1	2.73	0.42
4:D:485:ASN:O	4:D:486:HIS:C	2.57	0.42
4:D:420:MET:HA	4:D:425:ARG:O	2.20	0.42
4:D:685:VAL:HG13	4:D:686:SER:N	2.34	0.42
4:D:117:ILE:HG23	4:D:752:LEU:CD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:170:LEU:HD11	4:D:179:LYS:HB3	2.02	0.41
4:D:203:SER:C	4:D:205:HIS:H	2.23	0.41
4:D:533:PRO:HA	4:D:816:THR:O	2.20	0.41
4:D:747:LEU:HD23	4:D:755:PHE:O	2.20	0.41
1:T:120:DT:C2'	1:T:119:DT:OP2	2.53	0.41
4:D:143:ARG:HH11	4:D:143:ARG:HG2	1.85	0.41
4:D:219:MET:H	4:D:222:GLU:CG	2.34	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
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
1:T:115:DC:H4'	4:D:431:MET:HE2	2.01	0.41
4:D:40:GLU:OE2	4:D:286:TYR:HB3	2.20	0.41
4:D:506:ASP:N	4:D:506:ASP:OD2	2.43	0.41
4:D:54:MET:C	4:D:56:GLU:N	2.74	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:CD1	4:D:853:LEU:H	2.30	0.41
1:T:120:DT:H2'	1:T:120:DT:O5'	2.20	0.41
4:D:151:PHE:O	4:D:153:ARG:N	2.43	0.41
4:D:749:LEU:O	4:D:750:MET:HB2	2.20	0.41
4:D:424:GLY:O	4:D:792:ARG:NH1	2.54	0.41
4:D:268:PHE:HB3	4:D:286:TYR:OH	2.21	0.41
4:D:576:LYS:CE	4:D:576:LYS:HA	2.50	0.41
4:D:860:LYS:O	4:D:862:PRO:HD3	2.20	0.41
4:D:258:ALA:O	4:D:259:GLY:C	2.56	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:HD22	4:D:579:ASN:HA	1.70	0.41
4:D:19:ILE:HG23	4:D:19:ILE:O	2.20	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:789:SER:O	4:D:793:LYS:HB2	2.20	0.41
4:D:378:LYS:HE2	4:D:378:LYS:HB3	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:667:PHE:O	4:D:668:THR:C	2.59	0.40
1:T:126:DT:H2"	1:T:125:DG:OP2	2.21	0.40
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:274:PRO:HA	4:D:275:PRO:HD3	1.96	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:337:VAL:HG21	4:D:512:LEU:HD21	2.03	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:637:LEU:HD22	4:D:685:VAL:HG13	2.02	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 5

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
4	D	460	LEU

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Mol	Chain	Res	Type
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%)	630 (92%)	53 (8%)	12	33

All (53) 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	57	ARG
4	D	109	ILE
4	D	120	LYS
4	D	151	PHE
4	D	154	ILE
4	D	169	GLN
4	D	190	MET
4	D	215	ARG
4	D	232	GLN
4	D	242	GLU
4	D	257	ARG
4	D	281	ILE
4	D	310	ASP
4	D	311	VAL
4	D	325	ASN
4	D	335	LEU
4	D	350	GLU
4	D	362	MET
4	D	377	TRP
4	D	386	ARG
4	D	401	MET
4	D	402	LEU
4	D	419	ASN
4	D	423	ARG
4	D	433	ASN
4	D	443	LEU
4	D	472	LYS

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Mol	Chain	Res	Type
4	D	506	ASP
4	D	514	PHE
4	D	546	PHE
4	D	565	GLU
4	D	567	VAL
4	D	576	LYS
4	D	577	LYS
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	750	MET
4	D	756	ARG
4	D	793	LYS
4	D	816	THR
4	D	852	GLN
4	D	855	GLU
4	D	859	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	135	GLN
4	D	169	GLN
4	D	184	GLN
4	D	211	HIS
4	D	321	ASN
4	D	339	ASN
4	D	406	ASN
4	D	419	ASN
4	D	433	ASN
4	D	435	GLN
4	D	466	ASN

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Mol	Chain	Res	Type
4	D	485	ASN
4	D	488	ASN
4	D	579	ASN
4	D	592	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	799	HIS
4	D	852	GLN
4	D	854	HIS
4	D	871	ASN

5.3.3 RNA ⓘ

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 ⓘ

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 ⓘ

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	27,33,33	1.49	4 (14%)	31,52,52	2.12	7 (22%)

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	-	3/15/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	901	APC	PB-O3B	3.96	1.62	1.58
5	R	901	APC	PA-O2A	-3.24	1.48	1.56
5	R	901	APC	PB-O2B	-3.22	1.48	1.56
5	R	901	APC	O3'-C3'	-2.02	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	901	APC	C1'-N9-C4	7.72	140.21	126.64
5	R	901	APC	O1B-PB-C3A	-5.06	95.69	109.07
5	R	901	APC	O2A-PA-O1A	2.91	119.78	110.07
5	R	901	APC	O2B-PB-O1B	2.75	119.25	110.07
5	R	901	APC	O2B-PB-C3A	2.34	116.16	106.58
5	R	901	APC	O2G-PG-O1G	2.27	119.57	110.68
5	R	901	APC	C5-C6-N6	2.16	123.63	120.35

There are no chirality outliers.

All (3) torsion outliers are listed below:

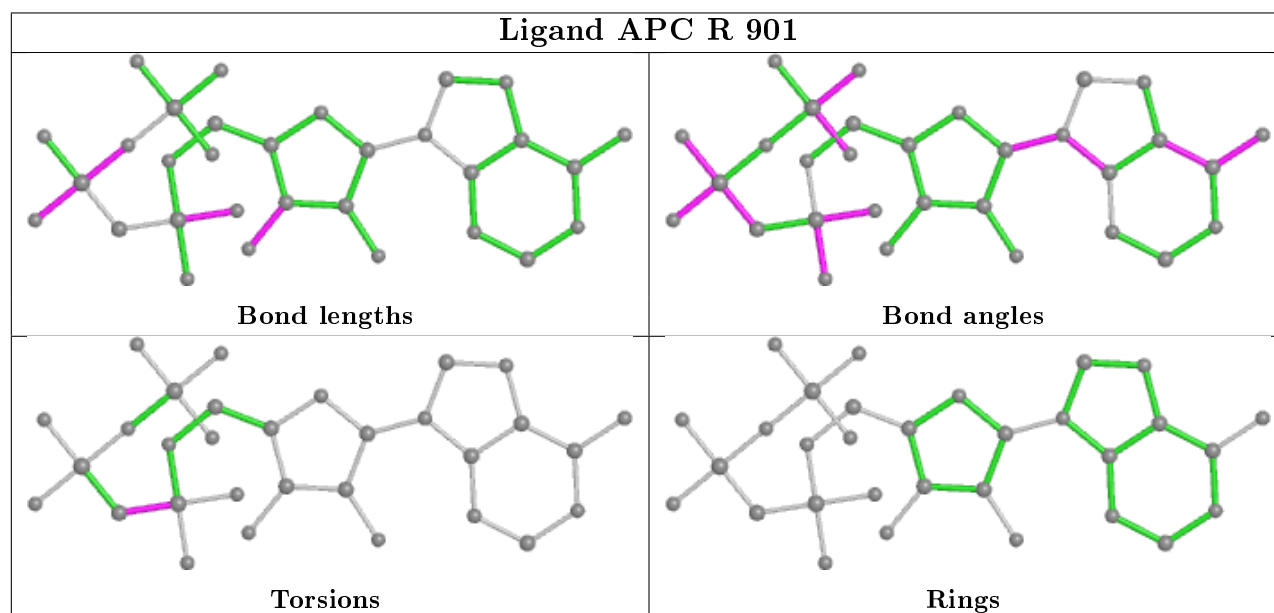
Mol	Chain	Res	Type	Atoms
5	R	901	APC	PB-C3A-PA-O1A
5	R	901	APC	PB-C3A-PA-O5'
5	R	901	APC	PB-C3A-PA-O2A

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 ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

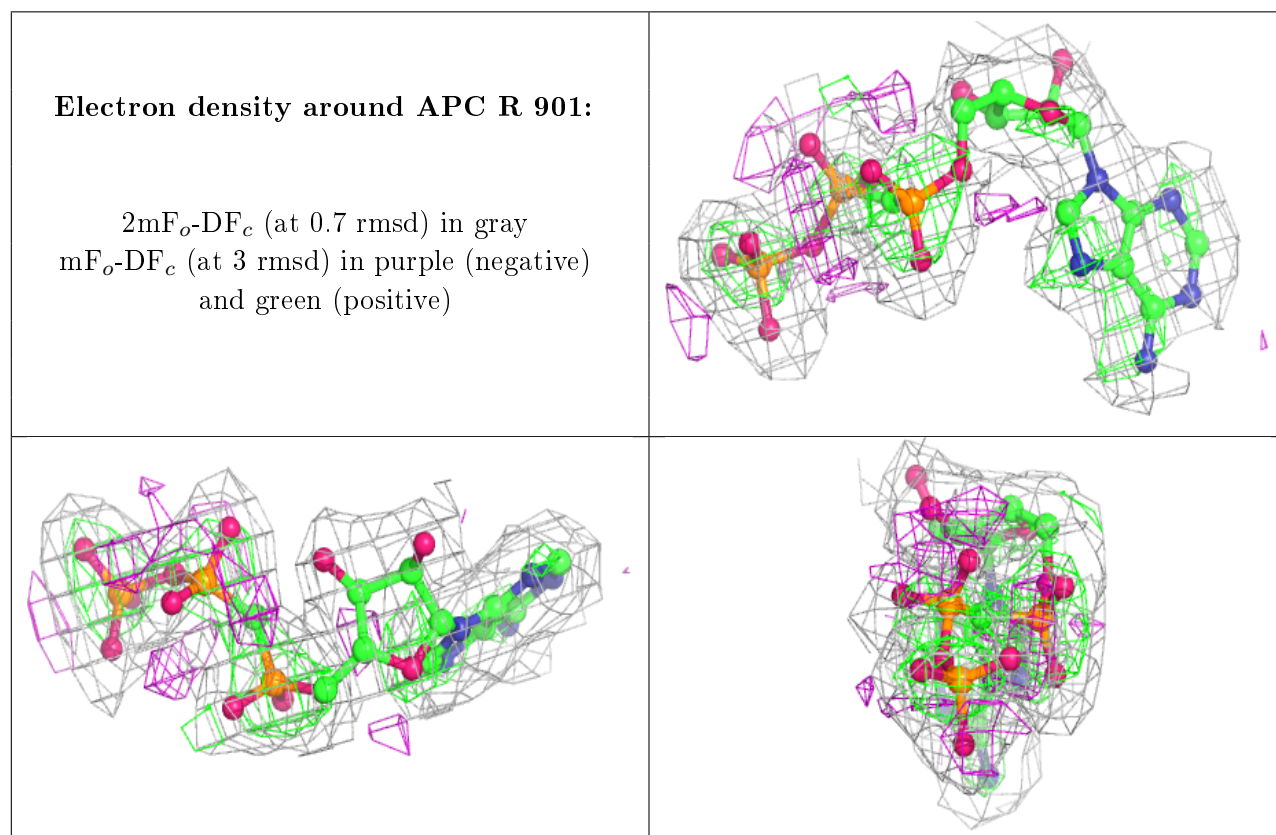
6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.