



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:08 PM UTC

PDB ID : 6UPY / pdb_00006upy
Title : RNA polymerase II elongation complex with 5-guanidinohydantoin lesion in state 2E
Authors : Oh, J.; Wang, D.
Deposited on : 2019-10-18
Resolution : 3.40 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

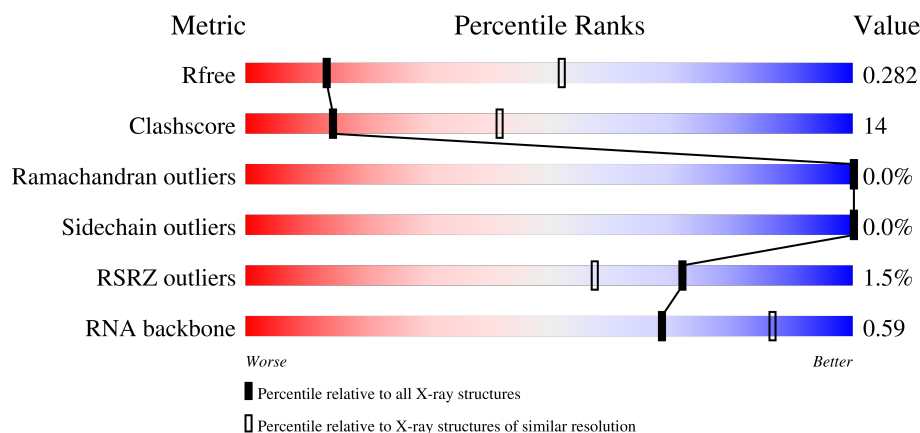
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



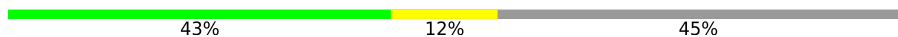
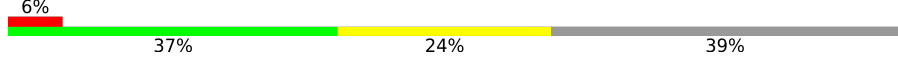
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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	R	9	67% 33%
2	T	29	38% 45% 14%
3	N	18	22% 61% 17%
4	A	1733	54% 25% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	L	70	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29013 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 RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	9	Total	C	N	O	P	0	0	0
			199	88	40	62	9			

- Molecule 2 is a DNA chain called Template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	25	Total	C	N	O	P	0	0	0
			500	239	78	158	25			

- Molecule 3 is a DNA chain called Non-template strand DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	15	Total	C	N	O	P	0	0	0
			317	148	71	83	15			

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1384	Total	C	N	O	S	0	0	0
			10851	6845	1898	2048	60			

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1109	Total	C	N	O	S	0	0	0
			8790	5566	1538	1633	53			

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	267	Total	C	N	O	S	0	0	0
			2101	1320	349	419	13			

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	213	Total	C	N	O	S	0	0	0
			1740	1104	307	318	11			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	86	Total	C	N	O	S	0	0	0
			684	437	115	129	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	133	Total	C	N	O	S	0	0	0
			1058	667	176	211	4			

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	117	Total	C	N	O	S	0	0	0
			945	581	172	182	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	43	Total	C	N	O	S	0	0	0
			337	208	66	59	4			

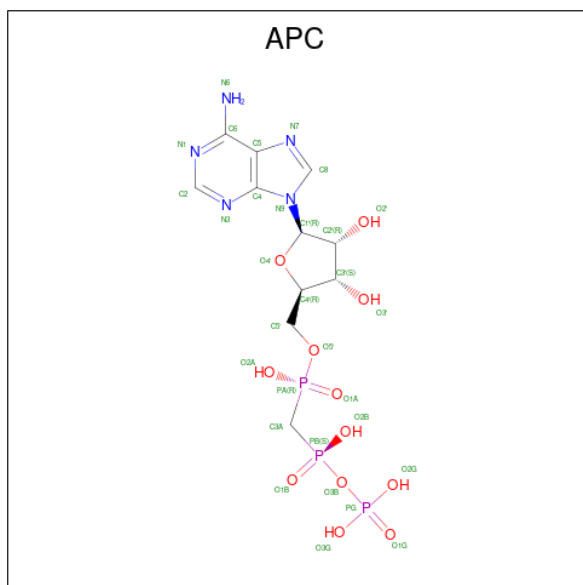
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		

- Molecule 16 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃) (labeled as "Ligand of Interest" by depositor).



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

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.

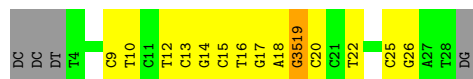
• Molecule 1: RNA

Chain R: 

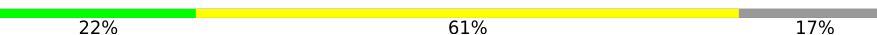


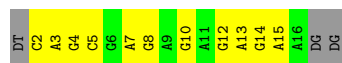
• Molecule 2: Template strand DNA

Chain T: 



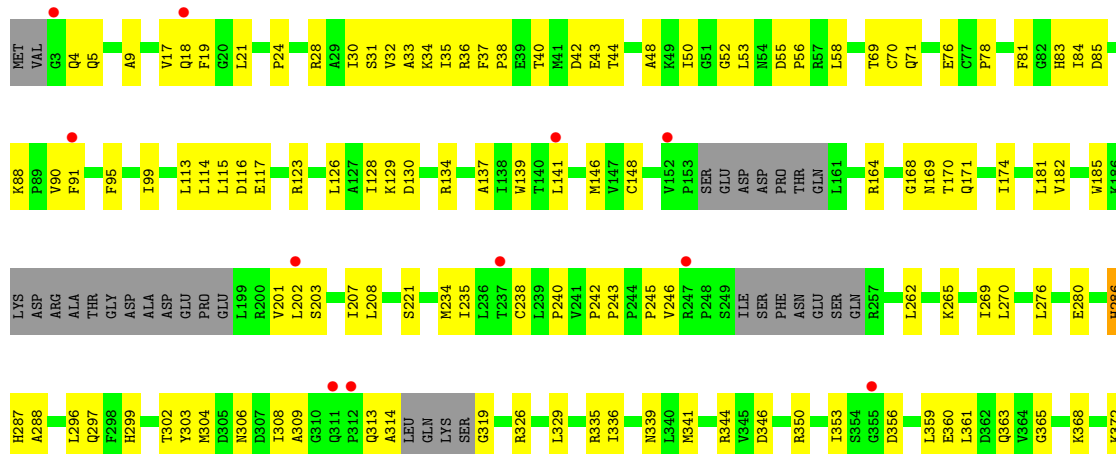
• Molecule 3: Non-template strand DNA

Chain N: 



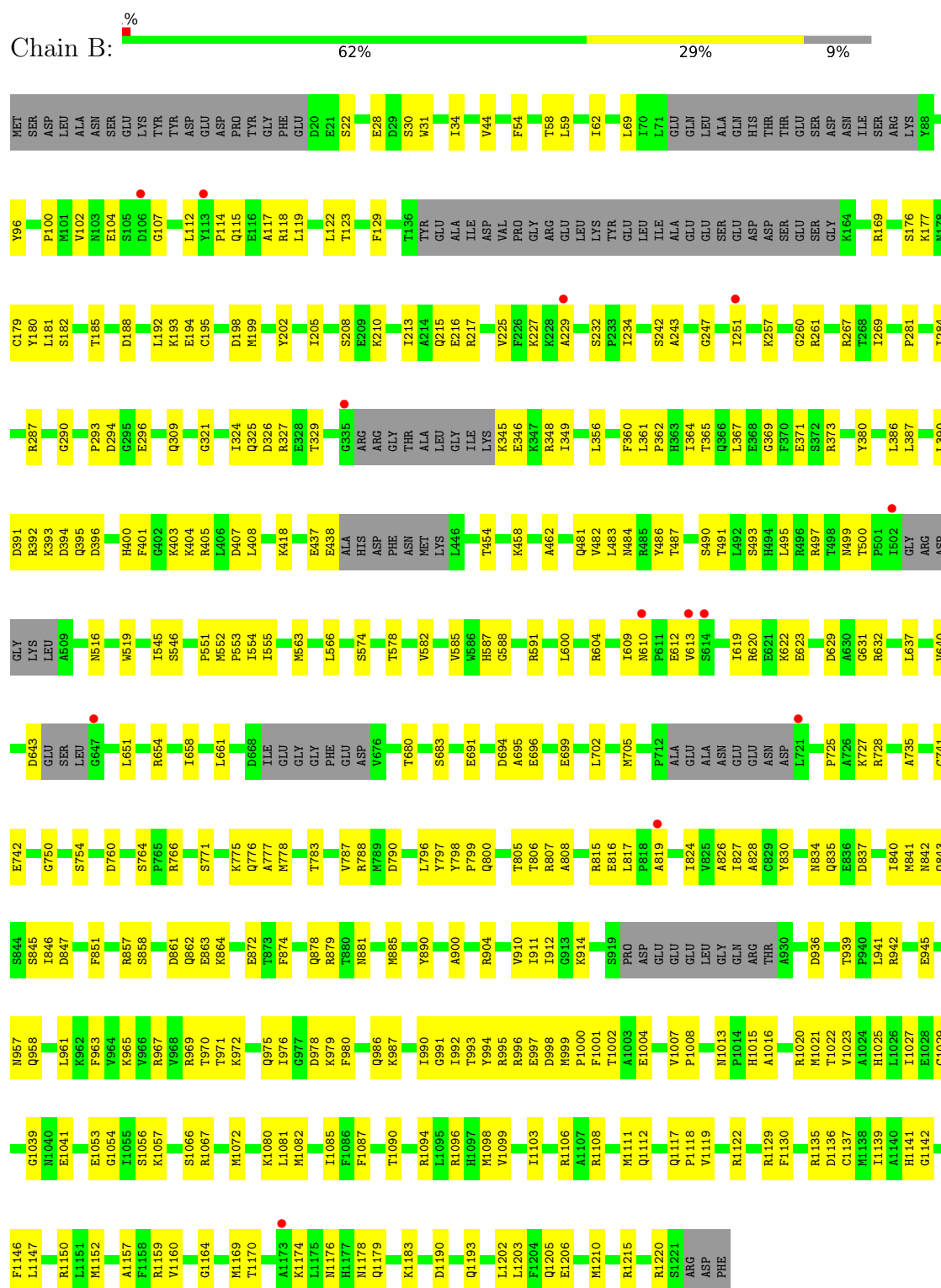
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

Chain A: 



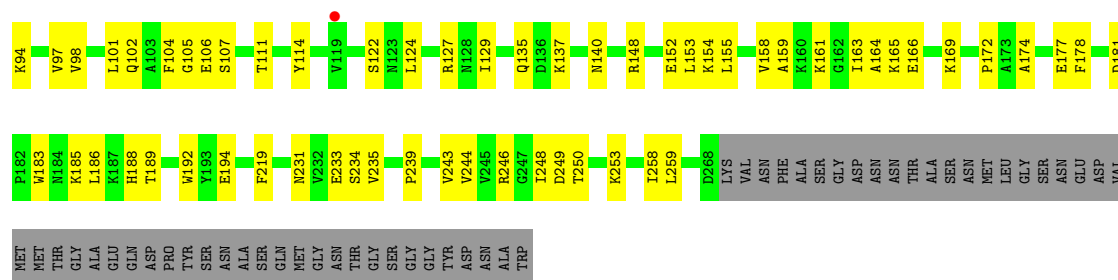
THR	SER	SER	PRO	THR	PRO	THR	THR	GLN	T1376	M1267	K1132	A1041	E932	Y836	V718	D592	F468	T373
SER	PRO	GLY	GLY	GLY	GLY	GLY	GLY	ASP	L1133	L1134	L1135	A1051	L936	I837	R731	T596	R469	L374
GLY	PRO	ALA	VAL	THR	THR	THR	THR	GLY	R1135	T1271	R1135	R1055	D939	K843	N736	L598	N471	T381
SER	SER	PRO	THR	THR	THR	THR	THR	THR	L1138	L1273	L1138	P1060	R940	V842	L737	S599	L472	Y382
PRO	PRO	SER	PRO	PRO	PRO	PRO	PRO	THR	V1276	E1277	T1161	G1061	D949	A844	K738	P600	V474	N384
GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1277	E1277	T1161	G1061	R944	E845	D739	R601	P477	R387
PRO	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	N1278	N1278	V1162	M1063	E945	E846	L740	D602	L388	L388
ALA	ALA	VAL	VAL	SER	SER	SER	SER	SER	P1164	P1164	V1065	G1065	V946	I848	N741	D483	D483	Y383
SER	SER	THR	THR	THR	THR	THR	THR	THR	V1291	P1292	V1165	V1065	D849	Y852	N742	L391	L391	N384
PRO	PRO	SER	SER	SER	SER	SER	SER	SER	D1166	D1166	L1167	L1067	D849	D853	K744	E486	E486	P386
ALA	ALA	VAL	VAL	VAL	VAL	VAL	VAL	VAL	I1169	I1169	L1176	A1068	P955	N854	K744	D609	M487	P386
GLN	GLN	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1176	L1176	L1176	I1072	L956	T856	M745	G610	V491	H399
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P957	T856	M745	G610	P400	P400
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	V958	T856	M745	G610	E500	E500
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	L1176	L1176	L1176	I1072	P958	T856	M745	G610	L501	L501
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	L1176	L1176	L1176	I1072	P958	T856	M745	G610	S502	S502
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	K403	K403
LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	LEU	L1176	L1176	L1176	I1072	P958	T856	M745	G610	I406	I406
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	R407	R407
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	L1176	L1176	L1176	I1072	P958	T856	M745	G610	D408	D408
VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	L1176	L1176	L1176	I1072	P958	T856	M745	G610	V507	V507
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	P508	P508
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	I413	I413
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	D414	D414
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	L415	L415
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	R416	R416
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	N517	N517
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	K518	K518
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	I424	I424
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	I523	I523
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	V524	V524
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	Q525	Q525
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	T527	T527
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	I531	I531
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	R532	R532
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	K533	K533
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	L534	L534
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	T535	T535
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	L536	L536
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	R537	R537
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	D544	D544
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	Q545	Q545
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	M549	M549
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	T566	T566
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	G574	G574
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	K575	K575
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	S579	S579
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	L710	L710
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	R711	R711
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	G585	G585
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	S466	S466
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	T467	T467
ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	L1176	L1176	L1176	I1072	P958	T856	M745	G610	H587	H587

● Molecule 5: DNA-directed RNA polymerase II subunit RPB2

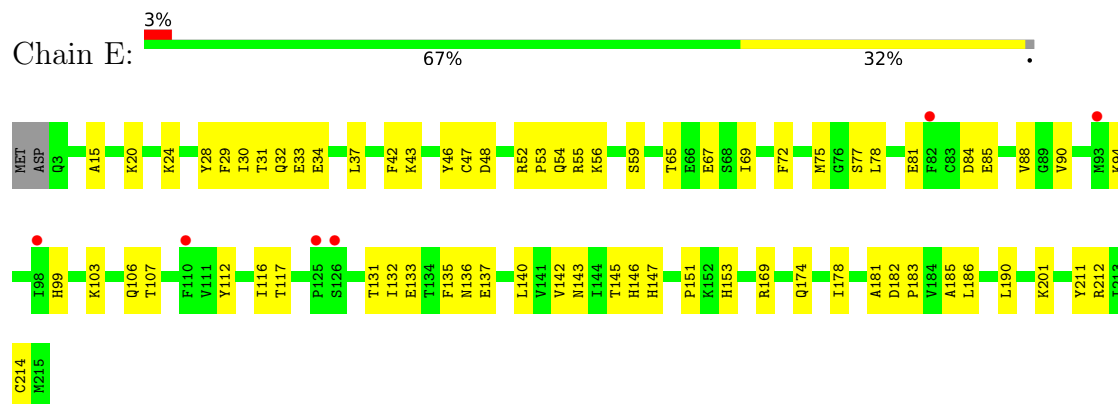


• Molecule 6: DNA-directed RNA polymerase II subunit RPB3

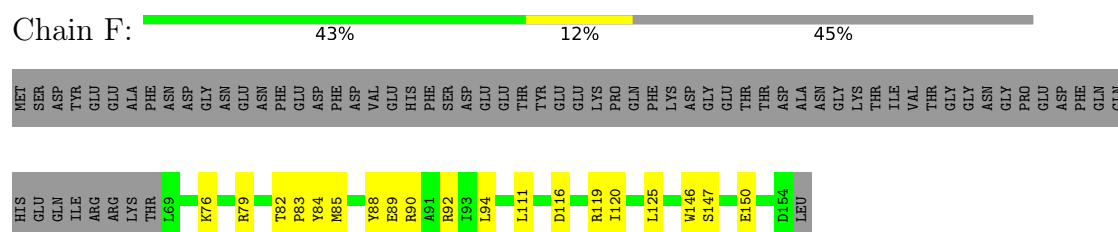




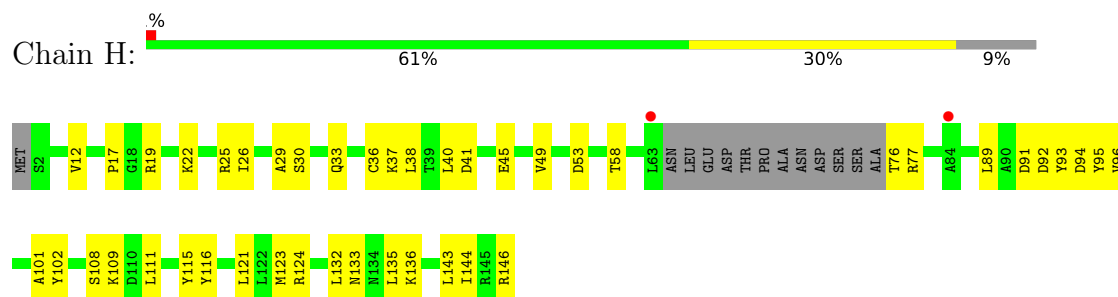
- Molecule 7: DNA-directed RNA polymerases I, II, and III subunit RPABC1



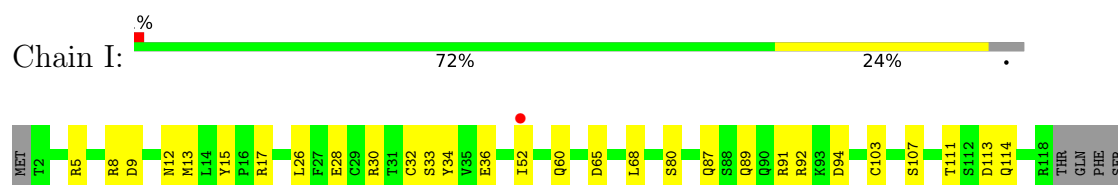
- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3



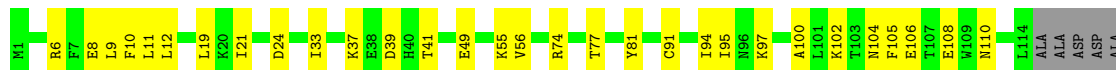
- Molecule 10: DNA-directed RNA polymerase II subunit RPB9



- Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

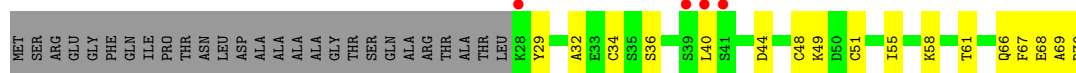


- Molecule 12: DNA-directed RNA polymerase II subunit RPB11



PHE

- Molecule 13: DNA-directed RNA polymerases I, II, and III subunit RPABC4



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.54Å 223.12Å 193.06Å 90.00° 100.92° 90.00°	Depositor
Resolution (Å)	49.22 – 3.40 49.22 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.22-3.40) 99.4 (49.22-3.40)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.227 , 0.282 0.229 , 0.282	Depositor DCC
R_{free} test set	2000 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	89.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 90.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29013	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: ZN, G35, 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	R	0.11	0/223	0.23	0/345
2	T	0.20	0/529	0.46	0/809
3	N	0.22	0/359	0.38	0/553
4	A	0.14	0/11042	0.39	2/14932 (0.0%)
5	B	0.13	0/8961	0.33	0/12090
6	C	0.12	0/2139	0.32	0/2899
7	E	0.13	0/1776	0.35	0/2391
8	F	0.12	0/696	0.33	0/943
9	H	0.13	0/1076	0.36	0/1459
10	I	0.13	0/963	0.38	0/1298
11	J	0.14	0/541	0.32	0/727
12	K	0.11	0/937	0.29	0/1265
13	L	0.21	0/339	0.61	0/450
All	All	0.14	0/29581	0.36	2/40161 (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
4	A	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1097	GLY	CA-C-N	5.06	123.43	120.24
4	A	1097	GLY	C-N-CA	5.06	123.43	120.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1106	ASN	Peptide
4	A	524	VAL	Peptide
4	A	566	ILE	Peptide

5.2 Too-close contacts [i](#)

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	R	199	0	98	7	0
2	T	500	0	287	16	0
3	N	317	0	166	11	0
4	A	10851	0	10916	348	0
5	B	8790	0	8781	272	0
6	C	2101	0	2056	84	0
7	E	1740	0	1761	54	0
8	F	684	0	692	14	0
9	H	1058	0	1018	34	0
10	I	945	0	890	27	0
11	J	532	0	543	32	0
12	K	919	0	929	24	0
13	L	337	0	352	13	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
16	B	31	0	14	2	0
All	All	29013	0	28503	804	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 14.

All (804) 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)
16:B:1301:APC:O4'	16:B:1301:APC:C1'	1.63	1.25
9:H:108:SER:HB2	9:H:111:LEU:HD13	1.21	1.15
4:A:451:HIS:CE1	4:A:1074:GLU:HG3	1.88	1.07
4:A:443:LEU:HD12	5:B:1146:PHE:CZ	2.01	0.95
9:H:109:LYS:O	9:H:111:LEU:HD12	1.77	0.85
4:A:326:ARG:HG3	4:A:1406:VAL:HG11	1.58	0.84
9:H:38:LEU:HD11	9:H:123:MET:HE2	1.60	0.83
4:A:269:ILE:HG22	4:A:299:HIS:HB3	1.60	0.82
4:A:848:ILE:HG21	4:A:1370:LEU:HD21	1.62	0.82
6:C:41:ILE:HG23	6:C:172:PRO:HG2	1.64	0.78
5:B:1099:VAL:HG12	5:B:1103:ILE:HD11	1.68	0.76
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.68	0.76
4:A:148:CYS:HB3	4:A:168:GLY:H	1.48	0.75
4:A:535:THR:O	4:A:575:LYS:NZ	2.19	0.75
4:A:859:SER:O	4:A:1422:ARG:NH1	2.20	0.74
4:A:982:THR:N	4:A:985:ASP:OD2	2.20	0.74
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.22	0.73
5:B:996:ARG:NH2	6:C:174:ALA:O	2.22	0.72
2:T:19:G35:H4'	2:T:19:G35:OP1	1.87	0.72
5:B:408:LEU:HD22	5:B:545:ILE:HD12	1.71	0.72
5:B:287:ARG:NH2	5:B:294:ASP:OD2	2.22	0.72
4:A:35:ILE:HD11	4:A:84:ILE:HB	1.69	0.72
6:C:94:LYS:HA	6:C:127:ARG:HH22	1.55	0.72
4:A:1325:THR:OG1	7:E:146:HIS:O	2.06	0.71
5:B:612:GLU:O	5:B:632:ARG:NH2	2.24	0.71
6:C:7:GLN:HB2	6:C:23:SER:HB2	1.73	0.71
11:J:9:SER:OG	11:J:48:ARG:NH2	2.23	0.71
5:B:796:LEU:HB3	5:B:799:PRO:HG3	1.72	0.70
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.23	0.70
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.25	0.70
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.20	0.70
4:A:896:ARG:HE	4:A:897:TYR:HE1	1.39	0.70
4:A:1363:VAL:HB	4:A:1368:MET:HE2	1.73	0.70
10:I:80:SER:OG	10:I:103:CYS:SG	2.50	0.70
4:A:360:GLU:OE2	4:A:651:LYS:NZ	2.23	0.70
4:A:852:TYR:HA	4:A:1060:PRO:HB3	1.74	0.70
7:E:46:TYR:HD2	7:E:53:PRO:HB3	1.56	0.70
5:B:552:MET:HG3	5:B:553:PRO:HD3	1.74	0.70
10:I:92:ARG:NH2	10:I:94:ASP:OD1	2.25	0.70
5:B:566:LEU:HD12	5:B:588:GLY:HA2	1.74	0.69
6:C:35:ARG:NH1	12:K:39:ASP:OD1	2.24	0.69
12:K:8:GLU:O	12:K:37:LYS:NZ	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:39:ALA:HA	6:C:164:ALA:HB3	1.72	0.69
11:J:7:CYS:HA	11:J:49:MET:HE3	1.73	0.69
1:R:9:G:OP1	5:B:987:LYS:NZ	2.23	0.69
4:A:1267:MET:HA	4:A:1271:ILE:HD13	1.75	0.69
5:B:904:ARG:NH2	13:L:68:GLU:OE2	2.25	0.69
5:B:519:TRP:HZ2	5:B:705:MET:HE1	1.57	0.69
4:A:846:GLU:OE2	4:A:1425:SER:OG	2.10	0.69
4:A:523:ILE:HG23	4:A:527:THR:HB	1.75	0.68
5:B:401:PHE:HA	5:B:404:LYS:HG3	1.74	0.68
5:B:62:ILE:HG23	5:B:418:LYS:HG2	1.75	0.68
11:J:10:CYS:SG	11:J:43:ARG:NE	2.66	0.68
6:C:66:ARG:NH1	11:J:3:VAL:O	2.18	0.68
7:E:133:GLU:HB3	7:E:135:PHE:HE1	1.58	0.68
4:A:43:GLU:HG2	4:A:44:THR:HG23	1.76	0.68
5:B:986:GLN:HG3	5:B:1025:HIS:HD2	1.57	0.68
4:A:566:ILE:HB	9:H:96:VAL:HB	1.76	0.67
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.76	0.67
6:C:69:LEU:O	11:J:6:ARG:NH2	2.26	0.67
4:A:78:PRO:O	5:B:1205:GLN:NE2	2.26	0.67
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.27	0.67
4:A:1132:LYS:HG2	4:A:1135:ARG:HH12	1.60	0.67
5:B:604:ARG:HD3	5:B:691:GLU:HG2	1.77	0.67
8:F:116:ASP:HB3	8:F:119:ARG:HB2	1.77	0.66
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.28	0.66
4:A:636:GLU:OE1	4:A:962:ARG:NH1	2.28	0.66
6:C:233:GLU:OE2	11:J:43:ARG:NH2	2.27	0.66
5:B:185:THR:OG1	5:B:188:ASP:OD1	2.12	0.66
4:A:997:LEU:O	4:A:1011:GLN:NE2	2.29	0.66
6:C:249:ASP:OD2	6:C:253:LYS:NZ	2.28	0.66
5:B:815:ARG:NH2	5:B:1041:GLU:OE2	2.30	0.65
4:A:1025:ARG:HA	4:A:1030:ARG:HH11	1.61	0.65
4:A:356:ASP:HB3	4:A:359:LEU:HB2	1.79	0.65
9:H:22:LYS:NZ	9:H:45:GLU:OE1	2.25	0.65
5:B:169:ARG:HB2	5:B:454:THR:HG23	1.79	0.65
4:A:1165:GLU:OE2	4:A:1194:ARG:NH2	2.30	0.65
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.29	0.65
5:B:287:ARG:NH1	5:B:324:ILE:O	2.29	0.64
4:A:286:HIS:CE1	4:A:288:ALA:HB3	2.32	0.64
6:C:258:ILE:HG23	12:K:19:LEU:HD11	1.79	0.64
4:A:1340:GLY:HA2	7:E:183:PRO:HD2	1.77	0.64
4:A:711:ARG:NH2	10:I:87:GLN:OE1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:886:ILE:HD11	4:A:943:LEU:HB2	1.80	0.64
5:B:260:GLY:O	5:B:267:ARG:NH1	2.28	0.64
5:B:766:ARG:HG2	5:B:1022:THR:HG22	1.80	0.64
4:A:91:PHE:HB2	4:A:297:GLN:HE22	1.62	0.64
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.80	0.64
4:A:668:ASP:O	4:A:741:ASN:ND2	2.30	0.64
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.79	0.64
5:B:620:ARG:HD2	10:I:68:LEU:HD11	1.80	0.64
6:C:54:ASN:OD1	6:C:56:THR:OG1	2.15	0.64
4:A:9:ALA:O	5:B:1193:GLN:NE2	2.29	0.64
7:E:107:THR:HA	7:E:131:THR:HB	1.80	0.64
4:A:472:LEU:HG	5:B:835:GLN:NE2	2.12	0.64
4:A:451:HIS:CE1	4:A:1074:GLU:CG	2.76	0.63
5:B:325:GLN:NE2	10:I:12:ASN:OD1	2.32	0.63
4:A:944:ARG:NH2	4:A:1296:GLY:O	2.28	0.63
2:T:10:DT:O2	3:N:10:DG:N2	2.32	0.63
4:A:407:ARG:HH11	4:A:413:ILE:HD11	1.62	0.63
5:B:193:LYS:HB3	5:B:787:VAL:HG11	1.79	0.63
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.80	0.63
4:A:879:GLU:OE1	4:A:962:ARG:NH2	2.29	0.63
4:A:69:THR:O	5:B:1174:LYS:NZ	2.31	0.63
7:E:28:TYR:HE1	7:E:78:LEU:HD13	1.62	0.63
9:H:29:ALA:HA	9:H:37:LYS:HA	1.81	0.62
2:T:14:DG:H1	3:N:5:DC:H42	1.47	0.62
12:K:100:ALA:O	12:K:104:ASN:ND2	2.32	0.62
6:C:88:CYS:HB3	6:C:92:CYS:HB3	1.82	0.62
5:B:28:GLU:OE2	5:B:807:ARG:NH2	2.24	0.62
4:A:313:GLN:HG3	4:A:314:ALA:H	1.65	0.62
5:B:365:THR:HG23	5:B:367:LEU:H	1.64	0.62
7:E:20:LYS:NZ	7:E:34:GLU:O	2.31	0.61
4:A:806:ARG:NH2	5:B:727:LYS:O	2.32	0.61
7:E:132:ILE:HD12	7:E:132:ILE:O	1.99	0.61
4:A:17:VAL:HG13	4:A:1419:ASP:HB3	1.81	0.61
4:A:443:LEU:HD12	5:B:1146:PHE:CE2	2.35	0.61
4:A:670:ILE:HD12	5:B:1067:ARG:HE	1.65	0.61
11:J:17:LYS:HB3	11:J:39:LEU:HD13	1.82	0.61
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.83	0.61
9:H:89:LEU:HD13	9:H:91:ASP:O	2.01	0.60
4:A:898:ARG:O	4:A:1029:ARG:NH1	2.34	0.60
5:B:22:SER:O	5:B:654:ARG:NH1	2.32	0.60
5:B:1053:GLU:OE2	5:B:1067:ARG:NH1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:33:ALA:HB1	4:A:56:PRO:HG2	1.82	0.60
5:B:828:ALA:O	5:B:834:ASN:ND2	2.33	0.60
4:A:18:GLN:HG2	5:B:1215:ARG:HB2	1.83	0.60
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.82	0.60
4:A:1002:GLY:O	4:A:1008:GLN:NE2	2.33	0.60
5:B:232:SER:O	5:B:261:ARG:NH2	2.33	0.60
5:B:620:ARG:HH11	10:I:68:LEU:HD21	1.66	0.60
6:C:47:ASP:OD2	13:L:70:ARG:NH1	2.34	0.60
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.35	0.60
5:B:393:LYS:HD3	10:I:89:GLN:HE22	1.67	0.60
4:A:1121:GLU:HB3	4:A:1124:HIS:HB2	1.84	0.60
4:A:901:LEU:HA	4:A:907:THR:HG23	1.83	0.60
4:A:81:PHE:CE2	4:A:240:PRO:HB2	2.37	0.59
4:A:50:ILE:HG12	4:A:52:GLY:H	1.66	0.59
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.31	0.59
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.83	0.59
12:K:106:GLU:O	12:K:110:ASN:ND2	2.29	0.59
4:A:890:ASP:OD1	4:A:940:ARG:NH1	2.36	0.59
5:B:841:MET:HE1	5:B:851:PHE:HD1	1.66	0.59
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.36	0.59
4:A:123:ARG:HA	4:A:126:LEU:HD12	1.85	0.59
4:A:738:LYS:NZ	6:C:194:GLU:O	2.35	0.59
5:B:373:ARG:HD3	5:B:566:LEU:HD22	1.84	0.59
5:B:483:LEU:HD21	5:B:491:THR:HG23	1.85	0.59
5:B:326:ASP:OD1	5:B:329:THR:OG1	2.20	0.59
6:C:93:ASP:OD1	6:C:122:SER:OG	2.20	0.59
9:H:146:ARG:HD2	9:H:146:ARG:H	1.68	0.59
10:I:17:ARG:N	10:I:26:LEU:O	2.33	0.59
4:A:527:THR:HG23	4:A:653:VAL:HB	1.84	0.59
4:A:913:LEU:HD22	4:A:915:SER:H	1.68	0.59
5:B:574:SER:HA	5:B:591:ARG:HH21	1.68	0.59
6:C:165:LYS:O	12:K:6:ARG:NH1	2.35	0.59
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.85	0.59
5:B:54:PHE:HA	5:B:58:THR:HB	1.84	0.58
5:B:971:THR:HB	6:C:61:GLU:OE1	2.03	0.58
5:B:486:TYR:HE2	5:B:778:MET:HG2	1.68	0.58
6:C:36:VAL:HG23	6:C:40:GLU:HB2	1.85	0.58
1:R:9:G:OP1	5:B:979:LYS:NZ	2.34	0.58
4:A:414:ASP:OD2	4:A:416:ARG:NH2	2.35	0.58
5:B:837:ASP:OD1	5:B:1020:ARG:NH2	2.36	0.58
4:A:24:PRO:HB3	4:A:238:CYS:HB3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:555:ILE:HD11	5:B:582:VAL:HG11	1.85	0.58
4:A:881:GLN:HA	4:A:961:ARG:HH22	1.68	0.58
4:A:1012:ARG:O	4:A:1016:THR:OG1	2.20	0.58
4:A:1329:THR:HG22	4:A:1331:SER:H	1.68	0.58
5:B:100:PRO:O	5:B:180:TYR:OH	2.19	0.58
6:C:40:GLU:HA	6:C:163:ILE:HG23	1.86	0.58
4:A:34:LYS:HB2	4:A:36:ARG:HH22	1.69	0.57
4:A:116:ASP:HB2	4:A:164:ARG:HH12	1.68	0.57
6:C:107:SER:OG	6:C:111:THR:OG1	2.21	0.57
5:B:213:ILE:O	5:B:215:GLN:NE2	2.38	0.57
4:A:575:LYS:HB3	4:A:612:ILE:HD11	1.85	0.57
4:A:973:ILE:O	9:H:136:LYS:NZ	2.37	0.57
11:J:13:VAL:O	11:J:17:LYS:NZ	2.37	0.57
4:A:1342:GLU:HG2	7:E:212:ARG:HH11	1.69	0.57
7:E:78:LEU:HD12	7:E:107:THR:HG21	1.86	0.57
4:A:381:THR:HG22	4:A:384:ASN:CG	2.30	0.57
5:B:986:GLN:HG3	5:B:1025:HIS:CD2	2.39	0.57
9:H:108:SER:CB	9:H:111:LEU:HD13	2.14	0.57
4:A:182:VAL:HG12	4:A:201:VAL:HA	1.87	0.57
6:C:135:GLN:NE2	6:C:235:VAL:O	2.37	0.57
7:E:143:ASN:ND2	7:E:145:THR:OG1	2.38	0.57
5:B:604:ARG:NH2	5:B:613:VAL:O	2.28	0.57
7:E:55:ARG:N	7:E:84:ASP:OD2	2.38	0.57
4:A:1438:THR:HG23	8:F:92:ARG:HD2	1.87	0.57
4:A:170:THR:HB	4:A:185:TRP:HD1	1.70	0.56
4:A:758:ILE:O	4:A:762:SER:OG	2.23	0.56
5:B:972:LYS:HD3	5:B:1098:MET:HE3	1.87	0.56
4:A:40:THR:HA	4:A:53:LEU:HD23	1.87	0.56
5:B:750:GLY:O	5:B:754:SER:OG	2.22	0.56
5:B:760:ASP:OD1	5:B:760:ASP:N	2.38	0.56
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.38	0.56
6:C:249:ASP:OD1	12:K:102:LYS:NZ	2.33	0.56
4:A:1118:VAL:HG22	4:A:1327:ILE:HD11	1.87	0.56
4:A:329:LEU:HA	4:A:335:ARG:H	1.70	0.56
8:F:94:LEU:HD21	8:F:125:LEU:HD13	1.87	0.56
4:A:525:GLN:O	5:B:1015:HIS:NE2	2.39	0.56
6:C:246:ARG:O	6:C:250:THR:OG1	2.22	0.56
6:C:69:LEU:HB3	11:J:6:ARG:HD2	1.88	0.56
13:L:32:ALA:HB3	13:L:55:ILE:HD13	1.87	0.56
4:A:537:ARG:NH2	9:H:41:ASP:OD2	2.39	0.56
5:B:117:ALA:HA	5:B:122:LEU:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:394:ASP:OD2	10:I:91:ARG:NH2	2.36	0.56
9:H:12:VAL:HG12	9:H:53:ASP:H	1.70	0.56
4:A:903:ASN:O	4:A:907:THR:OG1	2.19	0.56
4:A:1076:ALA:HA	4:A:1079:MET:HE2	1.88	0.56
4:A:1202:MET:HE1	4:A:1212:VAL:HG21	1.88	0.56
4:A:1021:LEU:HD11	4:A:1025:ARG:HH11	1.71	0.56
4:A:848:ILE:HG22	4:A:1064:VAL:HG23	1.88	0.55
5:B:651:LEU:HD21	5:B:741:CYS:HB3	1.87	0.55
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.86	0.55
5:B:176:SER:O	5:B:182:SER:OG	2.22	0.55
4:A:913:LEU:CD2	4:A:915:SER:H	2.20	0.55
11:J:48:ARG:O	11:J:52:THR:OG1	2.24	0.55
4:A:861:GLY:O	7:E:174:GLN:NE2	2.38	0.55
11:J:37:SER:HG	11:J:47:ARG:HH22	1.52	0.55
4:A:353:ILE:HD13	4:A:487:MET:HG3	1.88	0.55
4:A:457:ALA:HB3	4:A:506:ALA:HA	1.86	0.55
7:E:48:ASP:OD2	7:E:52:ARG:N	2.39	0.55
4:A:359:LEU:HD21	4:A:363:GLN:HB2	1.89	0.55
4:A:1397:LEU:HB2	4:A:1426:GLU:HG3	1.88	0.55
5:B:242:SER:HB2	5:B:362:PRO:HD2	1.88	0.55
6:C:163:ILE:HG22	6:C:165:LYS:H	1.71	0.55
5:B:1008:PRO:HB3	5:B:1087:PHE:HE1	1.72	0.55
4:A:302:THR:OG1	4:A:306:ASN:OD1	2.24	0.54
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.08	0.54
4:A:344:ARG:HB2	5:B:1118:PRO:HD2	1.88	0.54
4:A:1364:ASN:OD1	4:A:1366:ARG:NH1	2.39	0.54
7:E:56:LYS:NZ	7:E:85:GLU:OE2	2.40	0.54
4:A:336:ILE:HD11	5:B:1203:LEU:HD13	1.89	0.54
4:A:709:THR:HG22	4:A:711:ARG:H	1.73	0.54
5:B:857:ARG:NH1	5:B:945:GLU:OE2	2.40	0.54
6:C:166:GLU:HB2	12:K:10:PHE:HZ	1.72	0.54
9:H:40:LEU:HD13	9:H:123:MET:HB2	1.90	0.54
10:I:60:GLN:NE2	10:I:107:SER:OG	2.38	0.54
2:T:26:DG:H5''	5:B:482:VAL:HG11	1.90	0.54
4:A:287:HIS:O	4:A:287:HIS:ND1	2.41	0.54
5:B:824:ILE:HG22	5:B:1008:PRO:HA	1.89	0.54
6:C:186:LEU:HD13	6:C:188:HIS:CG	2.43	0.54
9:H:94:ASP:OD1	9:H:94:ASP:N	2.36	0.54
5:B:380:TYR:OH	5:B:623:GLU:OE2	2.18	0.54
4:A:129:LYS:HA	4:A:134:ARG:HH11	1.73	0.54
4:A:1195:LEU:HD11	4:A:1267:MET:HE3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:30:ILE:HG13	5:B:1170:THR:HG21	1.90	0.54
4:A:740:LEU:H	4:A:740:LEU:HD23	1.72	0.54
4:A:800:VAL:HG13	4:A:812:GLU:HB3	1.90	0.54
5:B:776:GLN:HB3	5:B:1096:ARG:HG2	1.90	0.53
7:E:181:ALA:HA	7:E:186:LEU:HD21	1.90	0.53
13:L:29:TYR:HE2	13:L:58:LYS:HE3	1.72	0.53
12:K:21:ILE:HD12	12:K:33:ILE:HG12	1.90	0.53
4:A:949:ASP:OD1	4:A:949:ASP:N	2.40	0.53
5:B:176:SER:OG	5:B:177:LYS:N	2.41	0.53
5:B:680:THR:O	5:B:683:SER:OG	2.22	0.53
5:B:978:ASP:OD2	5:B:1094:ARG:NH2	2.42	0.53
7:E:88:VAL:HG21	7:E:116:ILE:HG23	1.91	0.53
9:H:58:THR:HB	9:H:143:LEU:HB2	1.89	0.53
1:R:9:G:O6	2:T:20:DC:N4	2.42	0.53
4:A:37:PHE:HB2	4:A:52:GLY:HA3	1.91	0.53
4:A:455:MET:HE1	5:B:1130:PHE:HE1	1.73	0.53
5:B:694:ASP:OD2	5:B:695:ALA:N	2.41	0.53
11:J:6:ARG:HG2	11:J:13:VAL:HG12	1.89	0.53
2:T:9:DC:H2"	2:T:10:DT:H5"	1.90	0.53
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.90	0.53
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.42	0.53
7:E:106:GLN:O	7:E:131:THR:N	2.31	0.53
4:A:1297:GLU:OE1	4:A:1297:GLU:N	2.41	0.53
4:A:781:ASP:OD2	10:I:91:ARG:NH1	2.41	0.52
5:B:486:TYR:CE2	5:B:778:MET:HG2	2.45	0.52
5:B:843:GLN:HB2	5:B:993:THR:HB	1.91	0.52
10:I:34:TYR:CE2	10:I:36:GLU:HB3	2.43	0.52
5:B:862:GLN:HG2	5:B:963:PHE:HD1	1.74	0.52
7:E:116:ILE:HG22	7:E:117:THR:H	1.74	0.52
4:A:986:ILE:HD11	4:A:1032:LEU:HD21	1.91	0.52
4:A:1323:ASP:CG	4:A:1325:THR:HG22	2.34	0.52
4:A:424:ILE:HD12	4:A:424:ILE:O	2.09	0.52
4:A:635:ARG:HH12	4:A:877:HIS:CD2	2.28	0.52
4:A:683:ILE:HG21	4:A:801:GLU:HG3	1.91	0.52
5:B:1082:MET:HA	6:C:189:THR:HA	1.92	0.52
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.90	0.52
9:H:132:LEU:O	9:H:133:ASN:ND2	2.42	0.52
4:A:314:ALA:O	4:A:319:GLY:N	2.42	0.52
4:A:1215:ARG:O	4:A:1219:THR:OG1	2.28	0.52
5:B:1174:LYS:HB2	5:B:1179:GLN:HG3	1.92	0.52
4:A:888:GLY:O	4:A:940:ARG:NH2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1161:THR:OG1	4:A:1239:ARG:NH2	2.43	0.52
5:B:805:THR:OG1	5:B:1041:GLU:OE1	2.26	0.52
1:R:5:A:O2'	5:B:481:GLN:OE1	2.24	0.52
1:R:9:G:O2'	4:A:446:ARG:NH2	2.43	0.52
4:A:19:PHE:HE1	4:A:1396:ALA:HB3	1.74	0.52
4:A:148:CYS:HB3	4:A:168:GLY:N	2.21	0.52
4:A:848:ILE:HB	4:A:1065:GLY:HA3	1.90	0.52
5:B:790:ASP:O	5:B:858:SER:OG	2.25	0.52
5:B:941:LEU:HD13	5:B:942:ARG:N	2.25	0.52
10:I:8:ARG:HD2	10:I:9:ASP:N	2.25	0.52
4:A:453:MET:SD	4:A:453:MET:N	2.82	0.52
4:A:526:ASP:HB2	5:B:835:GLN:OE1	2.09	0.52
4:A:1441:PHE:CZ	8:F:89:GLU:HA	2.45	0.52
5:B:566:LEU:CD1	5:B:588:GLY:HA2	2.40	0.52
4:A:860:LEU:HA	4:A:1422:ARG:HH12	1.74	0.51
5:B:862:GLN:O	5:B:914:LYS:NZ	2.39	0.51
5:B:1080:LYS:NZ	6:C:181:ASP:O	2.39	0.51
7:E:185:ALA:HA	7:E:190:LEU:HD23	1.92	0.51
6:C:2:SER:OG	6:C:3:GLU:N	2.41	0.51
7:E:112:TYR:CD2	7:E:116:ILE:HD11	2.45	0.51
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.76	0.51
4:A:1076:ALA:HA	4:A:1079:MET:HG3	1.92	0.51
4:A:596:THR:HB	4:A:598:LEU:H	1.74	0.51
4:A:1276:VAL:HG21	4:A:1316:VAL:HG22	1.92	0.51
4:A:17:VAL:HG12	4:A:1421:CYS:SG	2.50	0.51
5:B:208:SER:OG	5:B:210:LYS:NZ	2.31	0.51
7:E:178:ILE:HG22	7:E:214:CYS:HA	1.91	0.51
4:A:946:VAL:HA	7:E:201:LYS:HE3	1.91	0.51
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.92	0.51
5:B:643:ASP:OD2	5:B:654:ARG:NH2	2.41	0.51
6:C:84:ARG:CZ	12:K:11:LEU:HD11	2.41	0.51
4:A:308:ILE:HG22	4:A:309:ALA:H	1.75	0.51
4:A:451:HIS:NE2	4:A:1074:GLU:HG3	2.22	0.51
6:C:93:ASP:O	6:C:127:ARG:NH2	2.43	0.51
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.93	0.51
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.44	0.51
4:A:765:VAL:HG13	4:A:800:VAL:HB	1.92	0.51
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	1.93	0.51
4:A:43:GLU:OE1	4:A:43:GLU:N	2.42	0.51
5:B:963:PHE:HZ	5:B:965:LYS:HE3	1.74	0.51
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.93	0.50
5:B:863:GLU:OE2	5:B:874:PHE:N	2.43	0.50
6:C:86:CYS:SG	6:C:87:PHE:N	2.84	0.50
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.46	0.50
4:A:778:GLY:HA3	5:B:516:ASN:HB2	1.92	0.50
5:B:115:GLN:HG2	5:B:193:LYS:HB2	1.92	0.50
5:B:437:GLU:HG2	5:B:438:GLU:HG3	1.93	0.50
5:B:1178:ASN:O	5:B:1178:ASN:ND2	2.44	0.50
9:H:95:TYR:HB3	9:H:144:ILE:HB	1.93	0.50
13:L:36:SER:OG	13:L:48:CYS:SG	2.58	0.50
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.30	0.50
9:H:76:THR:OG1	9:H:77:ARG:N	2.43	0.50
4:A:816:HIS:CG	5:B:764:SER:HG	2.29	0.50
4:A:1214:GLU:O	4:A:1218:GLN:OE1	2.30	0.50
5:B:851:PHE:HB3	5:B:1094:ARG:HD2	1.93	0.50
7:E:112:TYR:CG	7:E:116:ILE:HD11	2.47	0.50
8:F:147:SER:HB3	8:F:150:GLU:HG2	1.92	0.50
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.94	0.50
10:I:34:TYR:HE2	10:I:36:GLU:HB3	1.77	0.50
4:A:452:LYS:HG3	4:A:453:MET:SD	2.52	0.50
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.93	0.50
5:B:1152:MET:O	5:B:1157:ALA:HB2	2.12	0.50
11:J:57:ILE:HA	11:J:60:PHE:HD2	1.77	0.50
4:A:445:ASN:OD1	4:A:446:ARG:N	2.45	0.50
4:A:1121:GLU:HG3	4:A:1122:PRO:HD2	1.92	0.50
4:A:600:PRO:HA	9:H:25:ARG:NH1	2.26	0.50
11:J:37:SER:OG	11:J:47:ARG:NH2	2.32	0.50
4:A:306:ASN:O	4:A:306:ASN:ND2	2.45	0.50
11:J:45:CYS:O	11:J:48:ARG:NE	2.44	0.50
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.93	0.49
6:C:104:PHE:HD2	6:C:106:GLU:HG3	1.77	0.49
5:B:957:ASN:OD1	5:B:961:LEU:N	2.44	0.49
5:B:995:ARG:HH21	12:K:9:LEU:HD13	1.76	0.49
4:A:4:GLN:HE22	5:B:1159:ARG:H	1.60	0.49
4:A:1295:THR:HB	4:A:1297:GLU:OE1	2.12	0.49
7:E:67:GLU:OE1	7:E:67:GLU:N	2.36	0.49
4:A:365:GLY:HA3	4:A:469:ARG:HB2	1.95	0.49
4:A:408:ASP:OD1	4:A:430:TRP:NE1	2.33	0.49
4:A:531:ILE:O	4:A:535:THR:OG1	2.25	0.49
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.93	0.49
4:A:359:LEU:CD2	4:A:363:GLN:HB2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:281:PRO:HD2	5:B:284:ILE:HD12	1.94	0.49
5:B:546:SER:OG	5:B:631:GLY:N	2.45	0.49
5:B:999:MET:HG2	5:B:1007:VAL:HG22	1.95	0.49
5:B:1016:ALA:HA	5:B:1020:ARG:HH21	1.78	0.49
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.45	0.49
4:A:304:MET:SD	5:B:1210:MET:HG3	2.52	0.49
4:A:353:ILE:HG22	4:A:468:PHE:HB2	1.94	0.49
4:A:661:GLY:HA3	5:B:1081:LEU:HD22	1.95	0.49
5:B:188:ASP:O	5:B:192:LEU:HG	2.12	0.49
5:B:705:MET:HE3	5:B:742:GLU:HG3	1.95	0.49
5:B:123:THR:OG1	5:B:458:LYS:NZ	2.31	0.49
5:B:904:ARG:NH1	13:L:66:GLN:O	2.44	0.49
11:J:3:VAL:HG11	11:J:18:TRP:HB2	1.93	0.49
3:N:14:DG:O6	3:N:15:DA:N6	2.46	0.49
3:N:7:DA:H5"	4:A:139:TRP:CH2	2.47	0.49
5:B:247:GLY:O	5:B:418:LYS:NZ	2.39	0.49
5:B:890:TYR:CZ	5:B:910:VAL:HG21	2.48	0.48
6:C:2:SER:OG	12:K:104:ASN:OD1	2.31	0.48
11:J:41:LEU:HD11	11:J:50:ILE:HD12	1.94	0.48
4:A:21:LEU:HD21	4:A:95:PHE:CZ	2.48	0.48
4:A:374:LEU:C	4:A:436:ILE:HD13	2.38	0.48
4:A:585:GLY:N	4:A:609:ASP:OD1	2.44	0.48
5:B:225:VAL:H	5:B:396:ASP:HB2	1.76	0.48
4:A:113:LEU:HD13	4:A:115:LEU:O	2.13	0.48
5:B:405:ARG:HH11	5:B:632:ARG:HG2	1.78	0.48
6:C:32:SER:O	6:C:36:VAL:HG12	2.14	0.48
4:A:350:ARG:NE	4:A:486:GLU:OE2	2.44	0.48
4:A:1276:VAL:HB	4:A:1279:ILE:HG12	1.95	0.48
9:H:102:TYR:CZ	9:H:115:TYR:HB3	2.47	0.48
4:A:361:LEU:HA	4:A:471:ASN:HD22	1.79	0.48
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.45	0.48
4:A:701:LEU:HD21	10:I:114:GLN:HB2	1.96	0.48
4:A:808:LEU:O	5:B:728:ARG:NH1	2.47	0.48
5:B:216:GLU:OE1	5:B:500:THR:OG1	2.21	0.48
4:A:406:ILE:HB	4:A:431:LYS:HB2	1.95	0.48
4:A:534:LEU:O	4:A:574:GLY:HA3	2.13	0.48
4:A:630:ILE:HD12	4:A:630:ILE:H	1.79	0.48
6:C:31:ASN:O	6:C:35:ARG:HG3	2.14	0.48
6:C:69:LEU:HB2	11:J:5:VAL:HG21	1.96	0.48
7:E:46:TYR:CD2	7:E:53:PRO:HB3	2.43	0.48
5:B:114:PRO:HG3	5:B:181:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:911:ILE:HG22	5:B:912:ILE:HG13	1.95	0.48
3:N:2:DC:H4'	3:N:3:DA:OP1	2.14	0.48
4:A:353:ILE:HD12	4:A:470:LEU:HD21	1.95	0.48
5:B:861:ASP:OD1	5:B:914:LYS:NZ	2.36	0.48
6:C:101:LEU:HD23	6:C:155:LEU:HD11	1.96	0.48
6:C:174:ALA:HB3	6:C:233:GLU:HG2	1.96	0.48
4:A:128:ILE:HG23	4:A:134:ARG:HB3	1.96	0.47
5:B:346:GLU:HA	5:B:349:ILE:HD12	1.95	0.47
5:B:484:ASN:OD1	5:B:490:SER:OG	2.30	0.47
7:E:169:ARG:HH11	7:E:169:ARG:HB2	1.79	0.47
5:B:842:ASN:OD1	5:B:845:SER:N	2.37	0.47
6:C:57:VAL:HG21	11:J:60:PHE:CB	2.45	0.47
4:A:1422:ARG:HD3	5:B:1220:ARG:HH21	1.78	0.47
5:B:205:ILE:HG21	5:B:462:ALA:HB2	1.95	0.47
5:B:816:GLU:N	5:B:816:GLU:OE1	2.47	0.47
5:B:1007:VAL:HG22	5:B:1008:PRO:HD2	1.96	0.47
7:E:28:TYR:CE1	7:E:78:LEU:HD13	2.46	0.47
2:T:9:DC:H1'	2:T:10:DT:O4'	2.13	0.47
4:A:976:THR:OG1	4:A:977:LYS:NZ	2.47	0.47
6:C:169:LYS:NZ	13:L:69:ALA:O	2.44	0.47
5:B:563:MET:HE1	5:B:587:HIS:HB3	1.97	0.47
6:C:60:ASP:HB2	13:L:67:PHE:CZ	2.49	0.47
9:H:30:SER:OG	9:H:36:CYS:SG	2.60	0.47
5:B:1020:ARG:NH1	16:B:1301:APC:O2'	2.47	0.47
4:A:32:VAL:HG22	5:B:1183:LYS:HZ2	1.79	0.47
4:A:457:ALA:O	4:A:507:VAL:HG23	2.15	0.47
4:A:837:ILE:O	4:A:841:LEU:HG	2.15	0.47
4:A:881:GLN:NE2	4:A:958:VAL:O	2.36	0.47
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.95	0.47
5:B:800:GLN:OE1	11:J:52:THR:OG1	2.24	0.47
5:B:885:MET:HE2	5:B:890:TYR:CZ	2.49	0.47
6:C:46:ILE:HA	6:C:159:ALA:HA	1.96	0.47
8:F:111:LEU:HD12	8:F:111:LEU:O	2.14	0.47
4:A:169:ASN:ND2	4:A:170:THR:HG23	2.30	0.47
4:A:858:ASN:OD1	4:A:861:GLY:N	2.45	0.47
5:B:195:CYS:SG	5:B:783:THR:OG1	2.60	0.47
5:B:243:ALA:HB2	5:B:251:ILE:HA	1.97	0.47
5:B:390:LEU:HD13	5:B:392:ARG:NH2	2.30	0.47
4:A:353:ILE:HG21	4:A:487:MET:HG3	1.97	0.47
4:A:780:VAL:N	5:B:699:GLU:OE2	2.38	0.47
5:B:179:CYS:O	5:B:182:SER:OG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:629:ASP:O	5:B:632:ARG:NH1	2.46	0.47
6:C:8:VAL:O	12:K:108:GLU:HG3	2.15	0.47
4:A:381:THR:HG23	4:A:383:TYR:H	1.79	0.47
4:A:821:ARG:O	4:A:825:ILE:HG12	2.14	0.47
4:A:1068:ALA:O	4:A:1072:ILE:HG12	2.15	0.47
5:B:356:LEU:HA	5:B:360:PHE:HB3	1.96	0.47
5:B:1098:MET:HE2	5:B:1098:MET:HB2	1.83	0.47
9:H:41:ASP:HB3	9:H:121:LEU:HD22	1.96	0.47
5:B:1112:GLN:HG3	5:B:1119:VAL:HA	1.96	0.46
4:A:28:ARG:HH21	4:A:238:CYS:HB2	1.81	0.46
5:B:619:ILE:HD12	10:I:65:ASP:HB2	1.97	0.46
5:B:975:GLN:O	5:B:990:ILE:HD12	2.15	0.46
9:H:101:ALA:HB2	9:H:116:TYR:CE2	2.51	0.46
6:C:148:ARG:NH1	11:J:64:ASN:HA	2.30	0.46
4:A:28:ARG:NE	4:A:85:ASP:OD1	2.47	0.46
5:B:971:THR:HB	6:C:61:GLU:CD	2.40	0.46
6:C:244:VAL:O	6:C:248:ILE:HG13	2.15	0.46
4:A:900:ASP:O	4:A:907:THR:OG1	2.32	0.46
4:A:1111:MET:HE2	4:A:1111:MET:HB3	1.72	0.46
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.29	0.46
5:B:229:ALA:O	5:B:261:ARG:NH2	2.46	0.46
6:C:14:SER:N	6:C:17:ASN:O	2.49	0.46
6:C:16:ASP:OD1	6:C:16:ASP:N	2.46	0.46
6:C:41:ILE:HD12	6:C:246:ARG:HB3	1.96	0.46
7:E:43:LYS:HG2	7:E:47:CYS:SG	2.56	0.46
4:A:746:MET:SD	5:B:1015:HIS:ND1	2.89	0.46
5:B:360:PHE:CE2	5:B:361:LEU:HD13	2.51	0.46
4:A:513:SER:OG	4:A:518:LYS:O	2.28	0.46
4:A:1062:GLU:HG3	8:F:88:TYR:OH	2.15	0.46
5:B:658:ILE:HA	5:B:661:LEU:HD12	1.98	0.46
5:B:287:ARG:NH1	5:B:321:GLY:O	2.48	0.46
6:C:98:VAL:HG22	6:C:158:VAL:HG22	1.98	0.46
4:A:31:SER:C	5:B:1183:LYS:HZ1	2.22	0.46
4:A:901:LEU:O	4:A:920:LEU:HD23	2.16	0.46
5:B:309:GLN:NE2	10:I:52:ILE:HG21	2.30	0.46
5:B:519:TRP:CZ2	5:B:705:MET:HE1	2.46	0.46
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.97	0.46
2:T:19:G35:HN3	2:T:20:DC:H5	1.61	0.45
4:A:174:ILE:HD11	4:A:181:LEU:HD13	1.98	0.45
4:A:453:MET:HB3	4:A:477:PRO:HB2	1.98	0.45
4:A:881:GLN:HE22	4:A:958:VAL:C	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.16	0.45
5:B:487:THR:HG21	5:B:819:ALA:HB2	1.98	0.45
5:B:834:ASN:O	5:B:1013:ASN:HB2	2.16	0.45
6:C:183:TRP:HB2	6:C:185:LYS:HG3	1.98	0.45
8:F:116:ASP:O	8:F:120:ILE:HG12	2.16	0.45
11:J:1:MET:HB2	11:J:60:PHE:HE2	1.81	0.45
4:A:440:ASP:O	4:A:460:VAL:HG23	2.16	0.45
4:A:537:ARG:NH1	4:A:602:ASP:OD1	2.47	0.45
4:A:741:ASN:OD1	4:A:744:LYS:N	2.38	0.45
4:A:853:ASP:O	4:A:855:THR:N	2.44	0.45
5:B:387:LEU:HD23	5:B:387:LEU:HA	1.84	0.45
5:B:554:ILE:HD12	5:B:609:ILE:HD11	1.99	0.45
6:C:41:ILE:CD1	6:C:246:ARG:HB3	2.47	0.45
8:F:82:THR:HG22	8:F:84:TYR:H	1.80	0.45
11:J:57:ILE:HA	11:J:60:PHE:CD2	2.51	0.45
2:T:13:DC:H2"	2:T:14:DG:C8	2.52	0.45
4:A:446:ARG:HB2	4:A:487:MET:SD	2.57	0.45
11:J:1:MET:HE2	11:J:1:MET:HB3	1.87	0.45
12:K:49:GLU:OE2	12:K:97:LYS:NZ	2.38	0.45
3:N:12:DG:H2"	3:N:13:DA:C8	2.51	0.45
4:A:168:GLY:O	4:A:169:ASN:HB3	2.16	0.45
5:B:365:THR:OG1	5:B:367:LEU:HG	2.17	0.45
8:F:76:LYS:HG2	8:F:79:ARG:HH21	1.82	0.45
12:K:91:CYS:O	12:K:95:ILE:HG13	2.17	0.45
4:A:287:HIS:O	4:A:287:HIS:CG	2.69	0.45
5:B:198:ASP:OD2	5:B:202:TYR:OH	2.29	0.45
5:B:879:ARG:HA	5:B:885:MET:SD	2.56	0.45
4:A:181:LEU:HD12	4:A:181:LEU:O	2.16	0.45
4:A:408:ASP:OD1	4:A:408:ASP:N	2.47	0.45
4:A:452:LYS:HB2	5:B:1141:HIS:CE1	2.52	0.45
5:B:992:ILE:HG12	5:B:994:TYR:CE2	2.50	0.45
11:J:2:ILE:HG12	11:J:3:VAL:H	1.82	0.45
12:K:12:LEU:HD12	12:K:12:LEU:H	1.81	0.45
4:A:699:ALA:HB1	10:I:114:GLN:HG2	1.97	0.45
4:A:1325:THR:HA	7:E:147:HIS:HA	1.99	0.45
4:A:1436:ILE:HD13	5:B:1139:ILE:HG23	1.99	0.45
9:H:115:TYR:CE2	9:H:124:ARG:HG3	2.52	0.45
4:A:38:PRO:HB3	4:A:270:LEU:HD13	1.99	0.45
5:B:104:GLU:HB2	5:B:107:GLY:HA3	1.99	0.45
5:B:227:LYS:N	5:B:395:GLN:OE1	2.49	0.45
5:B:637:LEU:HD23	5:B:742:GLU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:9:G:H5''	4:A:483:ASP:OD1	2.16	0.45
4:A:1093:LYS:HE2	4:A:1093:LYS:HB3	1.78	0.45
5:B:1142:GLY:HA3	8:F:88:TYR:HE2	1.82	0.45
6:C:57:VAL:HG21	11:J:60:PHE:CG	2.52	0.45
6:C:105:GLY:HA3	6:C:148:ARG:O	2.17	0.45
4:A:399:HIS:CD2	4:A:400:PRO:HA	2.52	0.45
4:A:368:LYS:O	4:A:372:LYS:N	2.45	0.44
4:A:767:GLN:HB2	4:A:799:PHE:HD1	1.82	0.44
4:A:1109:LYS:H	4:A:1109:LYS:HG2	1.49	0.44
4:A:465:TYR:HB3	5:B:976:ILE:HG21	2.00	0.44
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.99	0.44
5:B:405:ARG:NH1	5:B:632:ARG:HG2	2.32	0.44
5:B:487:THR:OG1	5:B:777:ALA:O	2.34	0.44
5:B:878:GLN:HB2	5:B:881:ASN:HB2	1.99	0.44
4:A:806:ARG:NH1	5:B:725:PRO:O	2.46	0.44
5:B:1160:VAL:HG11	5:B:1169:MET:SD	2.57	0.44
12:K:56:VAL:HA	12:K:77:THR:HG22	1.97	0.44
2:T:15:DC:H2''	2:T:16:DT:O5'	2.16	0.44
4:A:600:PRO:HA	9:H:25:ARG:HH12	1.81	0.44
4:A:899:VAL:HG22	4:A:1029:ARG:HD2	1.99	0.44
5:B:912:ILE:HB	5:B:939:THR:HB	1.99	0.44
9:H:135:LEU:HD23	9:H:136:LYS:N	2.32	0.44
4:A:668:ASP:OD1	6:C:192:TRP:NE1	2.50	0.44
4:A:741:ASN:O	4:A:745:GLN:HG3	2.18	0.44
5:B:578:THR:HG23	5:B:622:LYS:C	2.41	0.44
5:B:797:TYR:O	11:J:1:MET:N	2.51	0.44
5:B:1106:ARG:NH2	5:B:1111:MET:SD	2.91	0.44
11:J:57:ILE:O	11:J:61:LEU:HG	2.18	0.44
13:L:40:LEU:HB3	13:L:44:ASP:CG	2.42	0.44
4:A:500:GLU:OE2	4:A:1438:THR:HG21	2.18	0.44
4:A:742:ASN:OD1	4:A:742:ASN:N	2.50	0.44
4:A:834:THR:HG21	4:A:1077:THR:HA	2.00	0.44
5:B:403:LYS:NZ	5:B:696:GLU:OE2	2.44	0.44
5:B:817:LEU:HD12	5:B:817:LEU:HA	1.80	0.44
7:E:31:THR:OG1	7:E:33:GLU:HG3	2.18	0.44
4:A:339:ASN:O	5:B:1117:GLN:NE2	2.47	0.44
4:A:971:PHE:CE1	4:A:1041:ALA:HA	2.53	0.44
4:A:1118:VAL:HA	4:A:1327:ILE:HG13	1.98	0.44
5:B:400:HIS:HB3	5:B:403:LYS:HG2	1.99	0.44
7:E:29:PHE:O	7:E:30:ILE:HD12	2.18	0.44
7:E:136:ASN:OD1	7:E:137:GLU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:3:DA:H2''	3:N:4:DG:H8	1.83	0.44
4:A:471:ASN:O	4:A:474:VAL:HG12	2.17	0.44
4:A:843:LYS:HA	4:A:843:LYS:HD2	1.79	0.44
4:A:1217:LYS:HD2	4:A:1228:TRP:CZ3	2.53	0.44
5:B:30:SER:O	5:B:34:ILE:HG13	2.18	0.44
5:B:54:PHE:O	5:B:59:LEU:N	2.51	0.44
4:A:55:ASP:HA	4:A:58:LEU:CB	2.48	0.44
4:A:70:CYS:HA	5:B:1174:LYS:HD3	1.99	0.44
4:A:146:MET:C	4:A:171:GLN:HB2	2.43	0.44
5:B:391:ASP:HB3	10:I:92:ARG:HG2	2.00	0.44
5:B:437:GLU:CD	5:B:437:GLU:H	2.26	0.44
7:E:72:PHE:HB2	7:E:75:MET:HB3	2.00	0.44
8:F:83:PRO:HA	8:F:146:TRP:CZ3	2.53	0.44
10:I:13:MET:HG3	10:I:15:TYR:CE1	2.53	0.44
10:I:111:THR:HG22	10:I:113:ASP:H	1.82	0.44
4:A:134:ARG:NH2	4:A:221:SER:O	2.49	0.43
5:B:215:GLN:OE1	5:B:499:ASN:HB3	2.16	0.43
5:B:969:ARG:NH1	6:C:61:GLU:HG2	2.32	0.43
4:A:95:PHE:O	4:A:99:ILE:N	2.43	0.43
4:A:866:PHE:CZ	7:E:211:TYR:HB2	2.53	0.43
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	2.00	0.43
7:E:78:LEU:HA	7:E:107:THR:HB	2.01	0.43
10:I:17:ARG:NE	10:I:28:GLU:OE1	2.51	0.43
3:N:2:DC:H2''	3:N:3:DA:O5'	2.19	0.43
4:A:836:TYR:OH	4:A:1403:GLU:OE2	2.17	0.43
4:A:1212:VAL:O	4:A:1216:ILE:HG13	2.18	0.43
5:B:705:MET:HE3	5:B:705:MET:HA	2.00	0.43
5:B:705:MET:CE	5:B:742:GLU:HG3	2.49	0.43
7:E:59:SER:HB3	7:E:81:GLU:HA	2.00	0.43
4:A:442:VAL:HG12	4:A:491:VAL:HG22	2.00	0.43
5:B:122:LEU:HD22	5:B:958:GLN:HG3	1.99	0.43
6:C:104:PHE:CD2	6:C:106:GLU:HG3	2.53	0.43
7:E:37:LEU:CD1	7:E:42:PHE:HB2	2.48	0.43
7:E:43:LYS:HE2	7:E:43:LYS:HB3	1.78	0.43
9:H:26:ILE:HD11	9:H:49:VAL:HG11	2.00	0.43
4:A:83:HIS:HA	4:A:240:PRO:HA	2.01	0.43
4:A:114:LEU:HB2	4:A:115:LEU:HD22	2.01	0.43
4:A:360:GLU:HB2	4:A:363:GLN:HG3	1.99	0.43
4:A:506:ALA:HB1	4:A:508:PRO:HD2	2.00	0.43
4:A:587:HIS:CE1	4:A:608:ILE:HD12	2.54	0.43
4:A:896:ARG:HB3	4:A:897:TYR:HD1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:842:ASN:O	5:B:846:ILE:HG12	2.18	0.43
6:C:219:PHE:CD2	9:H:45:GLU:HG2	2.53	0.43
7:E:133:GLU:HB3	7:E:135:PHE:CE1	2.46	0.43
3:N:13:DA:H2"	3:N:14:DG:C8	2.53	0.43
4:A:276:LEU:HD23	4:A:280:GLU:HG3	1.99	0.43
4:A:341:MET:HE2	4:A:1401:SER:HB2	2.00	0.43
4:A:533:LYS:HE2	4:A:533:LYS:HB3	1.82	0.43
4:A:842:VAL:HG11	5:B:1136:ASP:OD2	2.19	0.43
4:A:857:ARG:HB3	4:A:861:GLY:HA2	2.00	0.43
4:A:1392:SER:HB2	4:A:1394:THR:HG23	2.00	0.43
5:B:806:THR:HG22	5:B:808:ALA:H	1.84	0.43
5:B:1039:GLY:O	11:J:32:GLU:HB2	2.18	0.43
5:B:1164:GLY:HA3	5:B:1190:ASP:OD1	2.18	0.43
6:C:52:GLU:N	6:C:154:LYS:O	2.52	0.43
6:C:169:LYS:NZ	13:L:70:ARG:HG2	2.34	0.43
12:K:55:LYS:HB2	12:K:81:TYR:CE1	2.54	0.43
4:A:361:LEU:HD12	4:A:471:ASN:HD22	1.83	0.43
4:A:675:THR:O	4:A:679:ILE:HG12	2.18	0.43
4:A:1021:LEU:HD11	4:A:1025:ARG:HD2	2.00	0.43
6:C:10:ILE:HG12	6:C:20:PHE:HB3	2.01	0.43
6:C:104:PHE:CD1	6:C:152:GLU:HB3	2.54	0.43
7:E:15:ALA:HA	7:E:140:LEU:O	2.18	0.43
4:A:387:ARG:O	4:A:391:LEU:HG	2.19	0.43
4:A:596:THR:HG22	4:A:597:LEU:H	1.84	0.43
5:B:600:LEU:HD23	5:B:600:LEU:HA	1.89	0.43
6:C:57:VAL:HG21	11:J:60:PHE:HB3	1.99	0.43
5:B:345:LYS:HD2	5:B:348:ARG:NH2	2.32	0.43
5:B:1094:ARG:NH1	5:B:1098:MET:SD	2.86	0.43
7:E:65:THR:O	7:E:69:ILE:HG23	2.19	0.43
7:E:99:HIS:O	7:E:103:LYS:N	2.51	0.43
4:A:242:PRO:HB2	4:A:246:VAL:HG21	2.01	0.43
4:A:1132:LYS:HA	4:A:1135:ARG:NH1	2.34	0.43
4:A:1318:THR:HG22	7:E:142:VAL:HG22	2.01	0.43
5:B:1072:MET:HB2	5:B:1081:LEU:HD12	2.00	0.43
4:A:1051:ALA:O	4:A:1055:ARG:HG3	2.18	0.42
4:A:1327:ILE:O	7:E:147:HIS:NE2	2.48	0.42
4:A:137:ALA:O	4:A:141:LEU:HG	2.19	0.42
5:B:980:PHE:CE2	5:B:1094:ARG:HG3	2.54	0.42
6:C:244:VAL:HG11	12:K:105:PHE:CZ	2.54	0.42
4:A:71:GLN:NE2	5:B:1176:ASN:HB3	2.34	0.42
4:A:265:LYS:HG3	4:A:303:TYR:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:372:LYS:HA	4:A:435:HIS:CE1	2.54	0.42
4:A:1120:LEU:O	4:A:1323:ASP:HB2	2.18	0.42
5:B:1029:CYS:HG	5:B:1090:THR:HG1	1.53	0.42
6:C:102:GLN:HA	6:C:153:LEU:O	2.18	0.42
6:C:234:SER:HB2	6:C:243:VAL:HG21	2.01	0.42
5:B:976:ILE:HD11	5:B:991:GLY:O	2.19	0.42
4:A:90:VAL:HG11	4:A:296:LEU:HD23	2.02	0.42
4:A:731:ARG:HG2	4:A:755:PHE:CE1	2.55	0.42
4:A:1003:LYS:HE3	4:A:1003:LYS:HB2	1.89	0.42
4:A:1163:ILE:HG22	4:A:1166:ASP:H	1.85	0.42
5:B:364:ILE:HD13	5:B:585:VAL:HG13	2.01	0.42
5:B:551:PRO:O	5:B:555:ILE:HG12	2.19	0.42
5:B:1054:GLY:HA2	5:B:1057:LYS:HD2	2.01	0.42
3:N:3:DA:H3'	4:A:1110:ASN:HD21	1.84	0.42
4:A:113:LEU:HD12	4:A:113:LEU:O	2.20	0.42
4:A:129:LYS:HA	4:A:134:ARG:NH1	2.35	0.42
4:A:760:GLN:HA	4:A:765:VAL:HA	2.00	0.42
4:A:873:MET:HG3	4:A:957:PRO:HG3	2.01	0.42
5:B:418:LYS:HE2	5:B:418:LYS:HB3	1.89	0.42
5:B:1001:PHE:HE1	6:C:178:PHE:HB3	1.85	0.42
6:C:51:VAL:HG13	6:C:155:LEU:HB3	2.02	0.42
4:A:579:SER:HB2	4:A:611:GLN:HA	2.01	0.42
4:A:803:SER:H	4:A:806:ARG:HB2	1.84	0.42
4:A:886:ILE:HD13	4:A:886:ILE:HA	1.92	0.42
10:I:8:ARG:H	10:I:8:ARG:HG3	1.72	0.42
4:A:646:PHE:O	4:A:650:GLN:HG3	2.20	0.42
4:A:1032:LEU:O	4:A:1036:ARG:HD3	2.20	0.42
4:A:1425:SER:O	4:A:1429:ILE:HG12	2.20	0.42
4:A:18:GLN:HB3	4:A:1418:LEU:HG	2.01	0.42
4:A:1278:ASN:HB2	4:A:1312:ASN:HB2	2.01	0.42
5:B:199:MET:SD	5:B:199:MET:N	2.83	0.42
5:B:771:SER:O	5:B:775:LYS:HE3	2.20	0.42
5:B:970:THR:HG22	5:B:971:THR:O	2.20	0.42
5:B:1108:ARG:CZ	5:B:1108:ARG:HB3	2.50	0.42
6:C:51:VAL:HA	6:C:155:LEU:HB3	2.02	0.42
12:K:39:ASP:OD1	12:K:41:THR:OG1	2.34	0.42
4:A:1212:VAL:HG13	4:A:1273:LEU:HD11	2.02	0.41
4:A:1384:VAL:HA	4:A:1389:PHE:CD2	2.55	0.41
5:B:861:ASP:OD1	5:B:862:GLN:N	2.53	0.41
6:C:97:VAL:HG21	6:C:129:ILE:HG22	2.02	0.41
4:A:344:ARG:CZ	5:B:1129:ARG:HG3	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:592:ASP:OD2	4:A:592:ASP:N	2.49	0.41
4:A:690:VAL:HG22	4:A:718:VAL:HG13	2.01	0.41
4:A:880:LYS:HA	4:A:955:PRO:HA	2.02	0.41
4:A:915:SER:O	4:A:919:ILE:HB	2.20	0.41
4:A:1279:ILE:HD12	4:A:1308:THR:HG21	2.02	0.41
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	2.02	0.41
5:B:44:VAL:HG11	5:B:495:LEU:HD13	2.03	0.41
5:B:118:ARG:NH1	5:B:194:GLU:OE1	2.52	0.41
5:B:290:GLY:HA2	5:B:327:ARG:HD2	2.03	0.41
7:E:77:SER:OG	7:E:106:GLN:HB3	2.20	0.41
7:E:185:ALA:HB1	7:E:190:LEU:HB2	2.03	0.41
9:H:92:ASP:O	9:H:146:ARG:NH1	2.53	0.41
2:T:22:DT:OP1	5:B:1129:ARG:HB2	2.20	0.41
4:A:28:ARG:NH2	4:A:238:CYS:HB2	2.36	0.41
4:A:202:LEU:HD13	4:A:202:LEU:HA	1.91	0.41
4:A:1116:LEU:HD12	4:A:1328:TYR:O	2.20	0.41
5:B:640:VAL:HG22	5:B:651:LEU:HD23	2.03	0.41
2:T:16:DT:H2'	2:T:17:DG:C8	2.55	0.41
4:A:388:LEU:HD23	4:A:388:LEU:HA	1.92	0.41
4:A:979:SER:OG	4:A:980:ASP:N	2.53	0.41
5:B:845:SER:HB2	11:J:8:PHE:HB3	2.02	0.41
7:E:151:PRO:HD2	7:E:153:HIS:HE1	1.86	0.41
13:L:49:LYS:HE2	13:L:49:LYS:HB2	1.91	0.41
2:T:12:DT:H2''	2:T:13:DC:C5	2.55	0.41
2:T:17:DG:H5'	2:T:18:DA:OP2	2.21	0.41
5:B:493:SER:OG	5:B:497:ARG:NH2	2.49	0.41
6:C:124:LEU:HD23	6:C:124:LEU:HA	1.93	0.41
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.53	0.41
1:R:4:G:H2'	1:R:5:A:C8	2.56	0.41
4:A:117:GLU:HB2	4:A:123:ARG:HD3	2.02	0.41
4:A:130:ASP:O	4:A:134:ARG:HG2	2.20	0.41
4:A:537:ARG:HD2	4:A:602:ASP:CG	2.45	0.41
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	2.02	0.41
4:A:1094:VAL:HA	4:A:1113:THR:HG21	2.03	0.41
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.55	0.41
6:C:77:ILE:HG13	6:C:161:LYS:HE3	2.02	0.41
6:C:259:LEU:HD12	6:C:259:LEU:HA	1.88	0.41
9:H:30:SER:HB2	9:H:33:GLN:HB3	2.02	0.41
9:H:93:TYR:HB2	9:H:143:LEU:HD12	2.02	0.41
4:A:58:LEU:HD23	4:A:58:LEU:HA	1.83	0.41
4:A:88:LYS:HE3	4:A:88:LYS:HB2	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:830:LYS:O	4:A:834:THR:OG1	2.25	0.41
5:B:1072:MET:HG3	5:B:1085:ILE:HB	2.03	0.41
7:E:178:ILE:HG12	7:E:182:ASP:OD2	2.20	0.41
10:I:15:TYR:CD1	10:I:30:ARG:HG3	2.55	0.41
10:I:32:CYS:SG	10:I:33:SER:N	2.90	0.41
4:A:396:PRO:HB3	4:A:403:LYS:HG2	2.03	0.41
4:A:663:SER:O	4:A:742:ASN:ND2	2.49	0.41
4:A:842:VAL:HG11	5:B:1136:ASP:CG	2.46	0.41
4:A:932:GLU:O	4:A:936:LEU:HG	2.20	0.41
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.54	0.41
5:B:864:LYS:HG2	5:B:872:GLU:OE1	2.21	0.41
7:E:52:ARG:O	7:E:54:GLN:NE2	2.52	0.41
7:E:90:VAL:O	7:E:94:LYS:HG3	2.20	0.41
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.53	0.41
4:A:455:MET:HE1	5:B:1130:PHE:CE1	2.55	0.41
4:A:675:THR:HG1	4:A:736:ASN:CG	2.25	0.41
4:A:939:ASP:O	4:A:943:LEU:HG	2.21	0.41
4:A:1291:VAL:HG22	4:A:1292:PRO:HD2	2.02	0.41
5:B:826:ALA:HB2	5:B:1087:PHE:CE1	2.56	0.41
6:C:73:GLN:OE1	6:C:75:MET:N	2.52	0.41
9:H:17:PRO:O	9:H:19:ARG:N	2.53	0.41
4:A:203:SER:O	4:A:207:ILE:HG13	2.21	0.41
4:A:457:ALA:HB2	4:A:501:LEU:HB3	2.02	0.41
4:A:544:ASP:OD1	4:A:545:GLN:N	2.54	0.41
4:A:1134:ILE:O	4:A:1138:ILE:HG12	2.21	0.41
4:A:1214:GLU:HA	4:A:1217:LYS:HD3	2.02	0.41
4:A:1434:ALA:O	4:A:1436:ILE:N	2.54	0.41
5:B:115:GLN:O	5:B:119:LEU:HG	2.21	0.41
5:B:393:LYS:HD2	5:B:393:LYS:HA	1.92	0.41
5:B:702:LEU:HD21	5:B:735:ALA:HB1	2.03	0.41
4:A:30:ILE:HD12	4:A:30:ILE:HA	1.91	0.40
4:A:42:ASP:HB3	4:A:48:ALA:HB3	2.03	0.40
4:A:1106:ASN:O	4:A:1107:VAL:C	2.63	0.40
5:B:69:LEU:HD23	5:B:69:LEU:HA	1.93	0.40
5:B:234:ILE:HD12	5:B:257:LYS:HB2	2.02	0.40
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.55	0.40
5:B:841:MET:HG2	5:B:846:ILE:HD11	2.02	0.40
5:B:890:TYR:CE2	5:B:910:VAL:HG21	2.56	0.40
5:B:1202:LEU:O	5:B:1206:GLU:HG3	2.21	0.40
6:C:239:PRO:O	6:C:243:VAL:HG23	2.21	0.40
7:E:135:PHE:HD2	7:E:140:LEU:HD21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:34:CYS:SG	13:L:51:CYS:HB3	2.61	0.40
4:A:262:LEU:HD12	4:A:262:LEU:HA	1.91	0.40
4:A:676:MET:HE1	4:A:762:SER:O	2.21	0.40
4:A:709:THR:HG23	10:I:94:ASP:HA	2.03	0.40
4:A:1303:GLU:CD	4:A:1326:ARG:HH12	2.27	0.40
12:K:49:GLU:HG3	12:K:94:ILE:HG13	2.03	0.40
4:A:1428:VAL:HG22	5:B:1147:LEU:HD11	2.04	0.40
9:H:40:LEU:HD13	9:H:123:MET:HE3	2.04	0.40
2:T:12:DT:O2	3:N:8:DG:N2	2.55	0.40
4:A:21:LEU:HD23	4:A:21:LEU:HA	1.78	0.40
4:A:359:LEU:HD23	4:A:360:GLU:N	2.36	0.40
4:A:451:HIS:NE2	4:A:1074:GLU:CG	2.84	0.40
4:A:527:THR:O	4:A:531:ILE:HB	2.21	0.40
4:A:607:ILE:HG12	4:A:612:ILE:HG22	2.02	0.40
5:B:788:ARG:O	5:B:967:ARG:NH1	2.54	0.40
5:B:797:TYR:HB3	5:B:798:TYR:CD1	2.56	0.40
6:C:137:LYS:HE3	6:C:137:LYS:HB3	1.87	0.40
4:A:21:LEU:HD21	4:A:95:PHE:HZ	1.83	0.40
4:A:99:ILE:HD11	4:A:234:MET:HB3	2.03	0.40
4:A:449:SER:HB3	5:B:1137:CYS:SG	2.60	0.40
4:A:900:ASP:N	4:A:906:HIS:O	2.50	0.40
5:B:369:GLY:HA2	5:B:371:GLU:OE1	2.22	0.40
5:B:1099:VAL:O	5:B:1103:ILE:HG12	2.22	0.40
9:H:26:ILE:HD12	9:H:26:ILE:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	A	1368/1733 (79%)	1298 (95%)	69 (5%)	1 (0%)	48 78

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	B	1089/1224 (89%)	1043 (96%)	46 (4%)	0	100	100
6	C	265/318 (83%)	259 (98%)	6 (2%)	0	100	100
7	E	211/215 (98%)	204 (97%)	7 (3%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	123 (95%)	6 (5%)	0	100	100
10	I	115/122 (94%)	110 (96%)	5 (4%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	108 (96%)	4 (4%)	0	100	100
13	L	41/70 (59%)	36 (88%)	5 (12%)	0	100	100
All	All	3477/4173 (83%)	3326 (96%)	150 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	286	HIS

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	A	1200/1520 (79%)	1200 (100%)	0	100	100
5	B	955/1061 (90%)	954 (100%)	1 (0%)	88	89
6	C	235/274 (86%)	235 (100%)	0	100	100
7	E	194/197 (98%)	194 (100%)	0	100	100
8	F	73/137 (53%)	73 (100%)	0	100	100
9	H	115/128 (90%)	115 (100%)	0	100	100
10	I	109/116 (94%)	109 (100%)	0	100	100
11	J	60/65 (92%)	60 (100%)	0	100	100
12	K	99/102 (97%)	99 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3077/3657 (84%)	3076 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	B	827	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	64	ASN
4	A	225	ASN
4	A	313	GLN
4	A	358	ASN
4	A	515	GLN
4	A	587	HIS
4	A	654	ASN
4	A	767	GLN
4	A	877	HIS
4	A	935	GLN
4	A	1004	ASN
4	A	1124	HIS
5	B	115	GLN
5	B	309	GLN
5	B	538	ASN
5	B	590	HIS
5	B	800	GLN
5	B	1015	HIS
6	C	65	HIS
6	C	203	GLN
7	E	113	GLN
7	E	143	ASN
7	E	174	GLN
9	H	131	ASN
10	I	22	ASN
10	I	89	GLN
12	K	112	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	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 ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	G35	T	19	2	18,23,24	4.83	14 (77%)	18,33,36	1.93	3 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	G35	T	19	2	-	3/11/41/42	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	C2-N3	9.53	1.49	1.33
2	T	19	G35	O4'-C4'	7.93	1.62	1.45
2	T	19	G35	C3'-C4'	-6.74	1.35	1.53
2	T	19	G35	C8-N9	6.56	1.46	1.37
2	T	19	G35	C5-N7	6.40	1.46	1.37
2	T	19	G35	O4'-C1'	-5.50	1.30	1.42
2	T	19	G35	C8-N7	4.84	1.47	1.38
2	T	19	G35	C2-N12	4.71	1.49	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	O3'-C3'	3.83	1.51	1.43
2	T	19	G35	C4-N3	3.45	1.48	1.44
2	T	19	G35	O8-C8	-2.92	1.17	1.23
2	T	19	G35	C1'-N9	2.79	1.49	1.45
2	T	19	G35	O5-C5	-2.75	1.18	1.23
2	T	19	G35	C2-N11	-2.51	1.25	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	T	19	G35	O4'-C1'-N9	6.07	115.85	108.65
2	T	19	G35	C4'-O4'-C1'	-3.83	100.40	109.51
2	T	19	G35	O4'-C1'-C2'	-3.18	100.30	106.25

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	G35	C3'-C4'-C5'-O5'
2	T	19	G35	C4'-C5'-O5'-P
2	T	19	G35	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	G35	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 9 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	$\# Z > 2$
16	APC	B	1301	-	29,33,33	3.38	9 (31%)	44,52,52	2.11	13 (29%)

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
16	APC	B	1301	-	-	9/19/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1301	APC	O4'-C1'	9.44	1.63	1.42
16	B	1301	APC	PB-O3B	8.25	1.67	1.58
16	B	1301	APC	C2'-C1'	-7.03	1.31	1.53
16	B	1301	APC	O4'-C4'	-6.48	1.30	1.45
16	B	1301	APC	O2'-C2'	4.39	1.53	1.43
16	B	1301	APC	C6-N6	4.13	1.44	1.34
16	B	1301	APC	PB-O2B	-3.30	1.48	1.56
16	B	1301	APC	O3'-C3'	-2.46	1.36	1.43
16	B	1301	APC	C5-C4	-2.45	1.34	1.39

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1301	APC	N3-C2-N1	-5.66	120.02	128.58
16	B	1301	APC	N6-C6-N1	-4.98	107.28	118.38
16	B	1301	APC	C5-C4-N3	-4.87	120.01	126.72
16	B	1301	APC	N9-C8-N7	-4.28	107.86	113.94
16	B	1301	APC	C5-C6-N6	3.84	132.80	123.29
16	B	1301	APC	C2-N3-C4	3.36	120.04	111.83
16	B	1301	APC	PB-O3B-PG	-3.11	121.32	132.45
16	B	1301	APC	C5-N7-C8	2.98	108.13	103.45
16	B	1301	APC	N3-C4-N9	2.92	132.13	127.17
16	B	1301	APC	C4-N9-C8	2.37	108.23	105.74
16	B	1301	APC	C4-C5-N7	-2.34	107.91	110.58
16	B	1301	APC	C3'-C2'-C1'	2.07	105.38	101.46

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
16	B	1301	APC	C6-C5-C4	2.04	119.96	117.18

There are no chirality outliers.

All (9) torsion outliers are listed below:

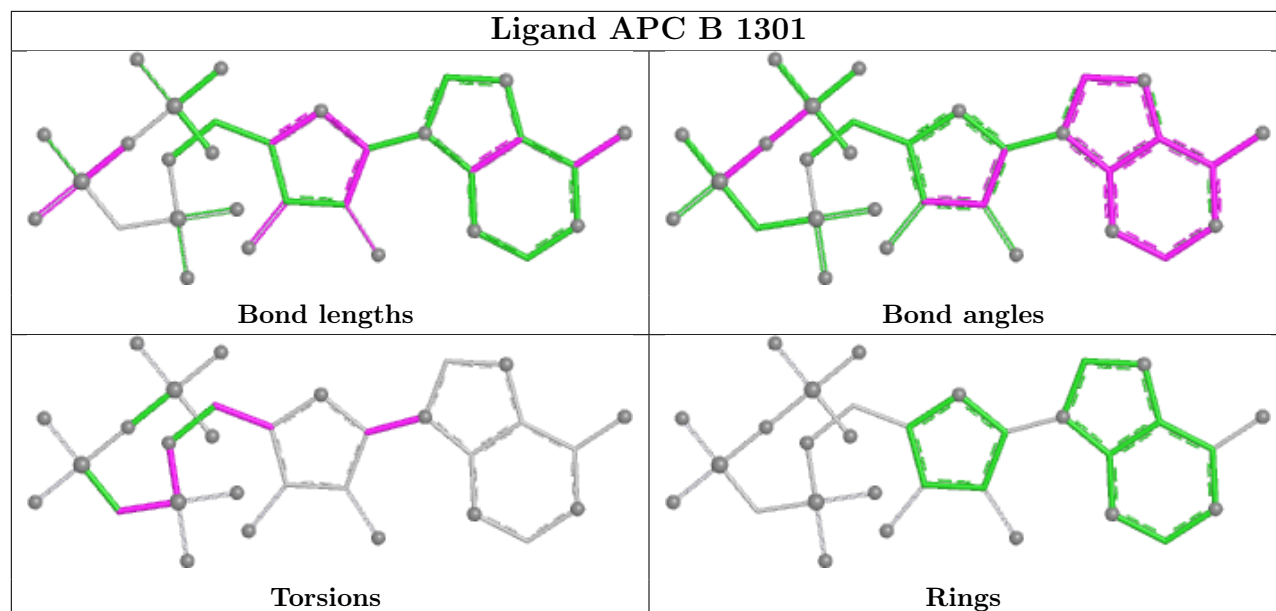
Mol	Chain	Res	Type	Atoms
16	B	1301	APC	PB-C3A-PA-O1A
16	B	1301	APC	PB-C3A-PA-O2A
16	B	1301	APC	PB-C3A-PA-O5'
16	B	1301	APC	O4'-C4'-C5'-O5'
16	B	1301	APC	C3'-C4'-C5'-O5'
16	B	1301	APC	C2'-C1'-N9-C8
16	B	1301	APC	C2'-C1'-N9-C4
16	B	1301	APC	C5'-O5'-PA-O2A
16	B	1301	APC	O4'-C1'-N9-C8

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1301	APC	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	R	9/9 (100%)	-0.49	0 100 100	89, 97, 145, 188	0
2	T	24/29 (82%)	-0.08	0 100 100	86, 171, 219, 235	0
3	N	15/18 (83%)	0.16	0 100 100	183, 203, 251, 254	0
4	A	1384/1733 (79%)	0.04	25 (1%) 67 53	51, 104, 184, 265	0
5	B	1109/1224 (90%)	-0.00	13 (1%) 76 63	32, 85, 153, 231	0
6	C	267/318 (83%)	-0.15	1 (0%) 88 81	56, 92, 138, 180	0
7	E	213/215 (99%)	0.15	6 (2%) 55 41	85, 140, 236, 292	0
8	F	86/155 (55%)	-0.17	0 100 100	66, 107, 149, 209	0
9	H	133/146 (91%)	0.05	2 (1%) 72 57	82, 125, 183, 224	0
10	I	117/122 (95%)	-0.08	1 (0%) 81 68	73, 106, 144, 167	0
11	J	65/70 (92%)	-0.09	1 (1%) 72 57	42, 73, 127, 145	0
12	K	114/120 (95%)	-0.30	0 100 100	62, 93, 131, 180	0
13	L	43/70 (61%)	0.71	4 (9%) 14 14	58, 146, 220, 268	0
All	All	3579/4229 (84%)	0.01	53 (1%) 72 57	32, 100, 186, 292	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	647	GLY	4.6
4	A	91	PHE	4.5
5	B	335	GLY	3.9
7	E	98	ILE	3.7
5	B	721	LEU	3.1
7	E	110	PHE	3.1
4	A	776	ALA	3.0
4	A	312	PRO	2.9
4	A	237	THR	2.9

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Mol	Chain	Res	Type	RSRZ
7	E	93	MET	2.9
9	H	63	LEU	2.8
4	A	18	GLN	2.8
5	B	819	ALA	2.8
5	B	1173	ALA	2.8
7	E	125	PRO	2.6
4	A	311	GLN	2.6
4	A	141	LEU	2.6
11	J	65	PRO	2.5
13	L	39	SER	2.5
7	E	126	SER	2.5
6	C	119	VAL	2.5
10	I	52	ILE	2.4
5	B	251	ILE	2.4
7	E	82	PHE	2.4
4	A	202	LEU	2.4
13	L	40	LEU	2.4
5	B	502	ILE	2.4
4	A	1315	GLU	2.4
4	A	1328	TYR	2.4
5	B	113	TYR	2.4
4	A	1332	PHE	2.3
5	B	229	ALA	2.3
4	A	844	ALA	2.3
4	A	1106	ASN	2.3
4	A	982	THR	2.2
13	L	41	SER	2.2
4	A	957	PRO	2.2
4	A	247	ARG	2.2
4	A	614	PHE	2.2
4	A	1176	LEU	2.1
5	B	106	ASP	2.1
13	L	28	LYS	2.1
9	H	84	ALA	2.1
5	B	614	SER	2.1
4	A	587	HIS	2.1
4	A	852	TYR	2.1
4	A	466	SER	2.0
4	A	3	GLY	2.0
4	A	449	SER	2.0
5	B	610	ASN	2.0
4	A	355	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
4	A	152	VAL	2.0
5	B	613	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	G35	T	19	22/23	0.80	0.16	138,155,172,184	0

6.3 Carbohydrates [i](#)

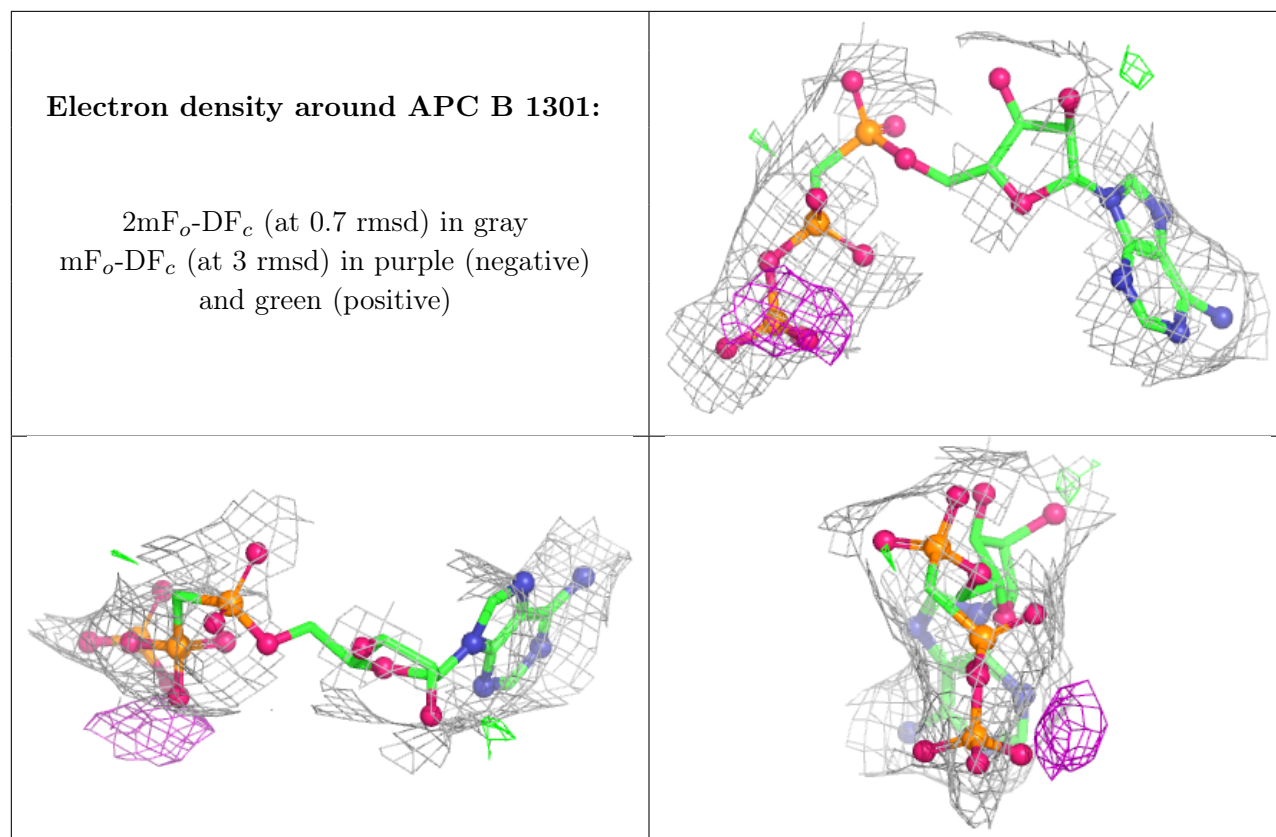
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	APC	B	1301	31/31	0.70	0.14	131,160,243,251	0
14	ZN	A	1801	1/1	0.94	0.06	393,393,393,393	0
14	ZN	L	101	1/1	0.95	0.07	231,231,231,231	0
14	ZN	A	1802	1/1	0.98	0.04	102,102,102,102	0
14	ZN	I	201	1/1	0.99	0.06	110,110,110,110	0
14	ZN	B	1302	1/1	0.99	0.03	209,209,209,209	0
15	MG	A	1803	1/1	0.99	0.02	39,39,39,39	0
14	ZN	C	401	1/1	0.99	0.03	131,131,131,131	0
14	ZN	J	101	1/1	1.00	0.05	79,79,79,79	0
14	ZN	I	202	1/1	1.00	0.02	80,80,80,80	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.