



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:56 AM UTC

PDB ID : 4A3E / pdb_00004a3e
Title : RNA Polymerase II initial transcribing complex with a 5nt DNA-RNA hybrid and soaked with AMPCPP
Authors : Cheung, A.C.M.; Sainsbury, S.; Cramer, P.
Deposited on : 2011-09-30
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

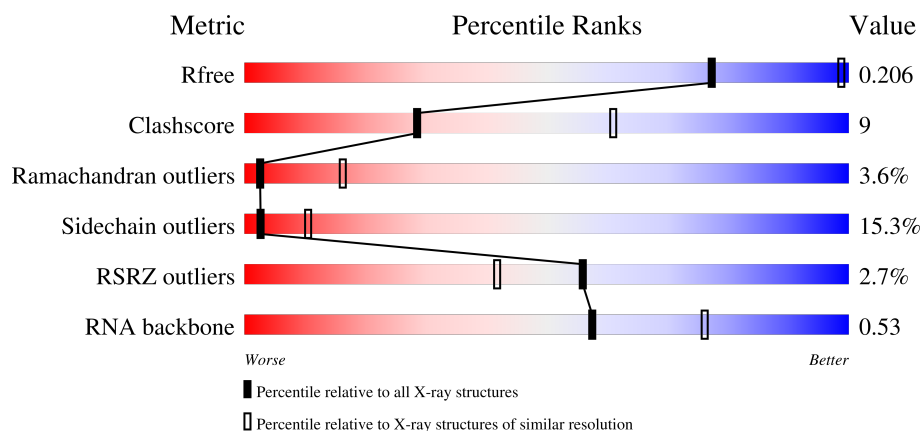
1 Overall quality at a glance

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	A	1732	52% 23% 6% 18%
2	B	1224	3% 60% 25% 5% 9%
3	C	318	56% 22% 5% 16%
4	D	221	5% 52% 21% 6% 19%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	 2% 65% 30% 5%
6	F	155	 37% 11% 6% 46%
7	G	171	 64% 26% 9%
8	H	146	 5% 62% 22% 5% 9%
9	I	122	 7% 66% 27%
10	J	70	 3% 46% 34% 13% 7%
11	K	120	 59% 33%
12	L	70	 7% 23% 29% 10% 34%
13	N	14	 29% 29% 29% 43%
14	P	5	 60% 20% 20%
15	T	26	 15% 23% 46% 31%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 31855 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1423	Total	C	N	O	S	0	0	0
			11182	7043	1955	2122	62			

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1115	Total	C	N	O	S	0	0	0
			8859	5609	1554	1641	55			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	178	Total	C	N	O	S	0	0	0
			1434	887	257	288	2			

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 7 is a protein called RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

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

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	115	Total	C	N	O	S	0	0	1
			920	590	157	171	2			

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

- Molecule 13 is a DNA chain called NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP *GP*CP*TP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	N	8	Total	C	N	O	P	0	0	0
			165	79	29	49	8			

- Molecule 14 is a RNA chain called TRANSCRIPT RNA 5'-R(*CP*AP*GP*GP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	P	4	Total	C	N	O	P	0	0	0
			90	40	20	26	4			

- Molecule 15 is a DNA chain called TEMPLATE DNA 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP *TP*TP*TP*CP*CP*BRU*GP*GP*TP*CP*AP*TP*TP)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
15	T	18	Total	Br	C	N	O	P	0	0	0
			365	1	175	58	113	18			

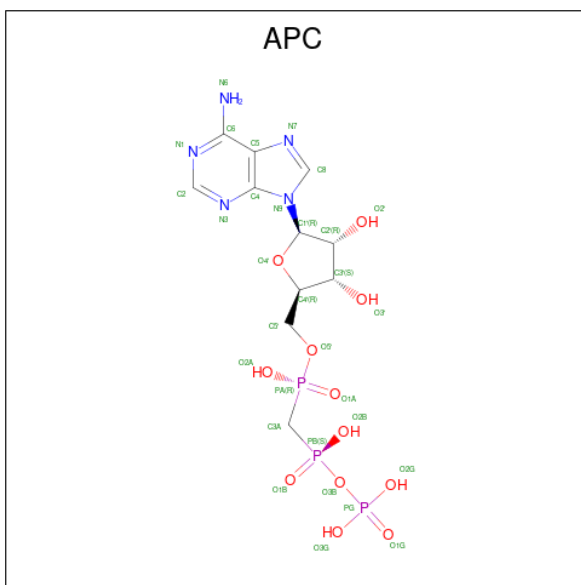
- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 18 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (CCD ID: APC) (formula: C₁₁H₁₈N₅O₁₂P₃).

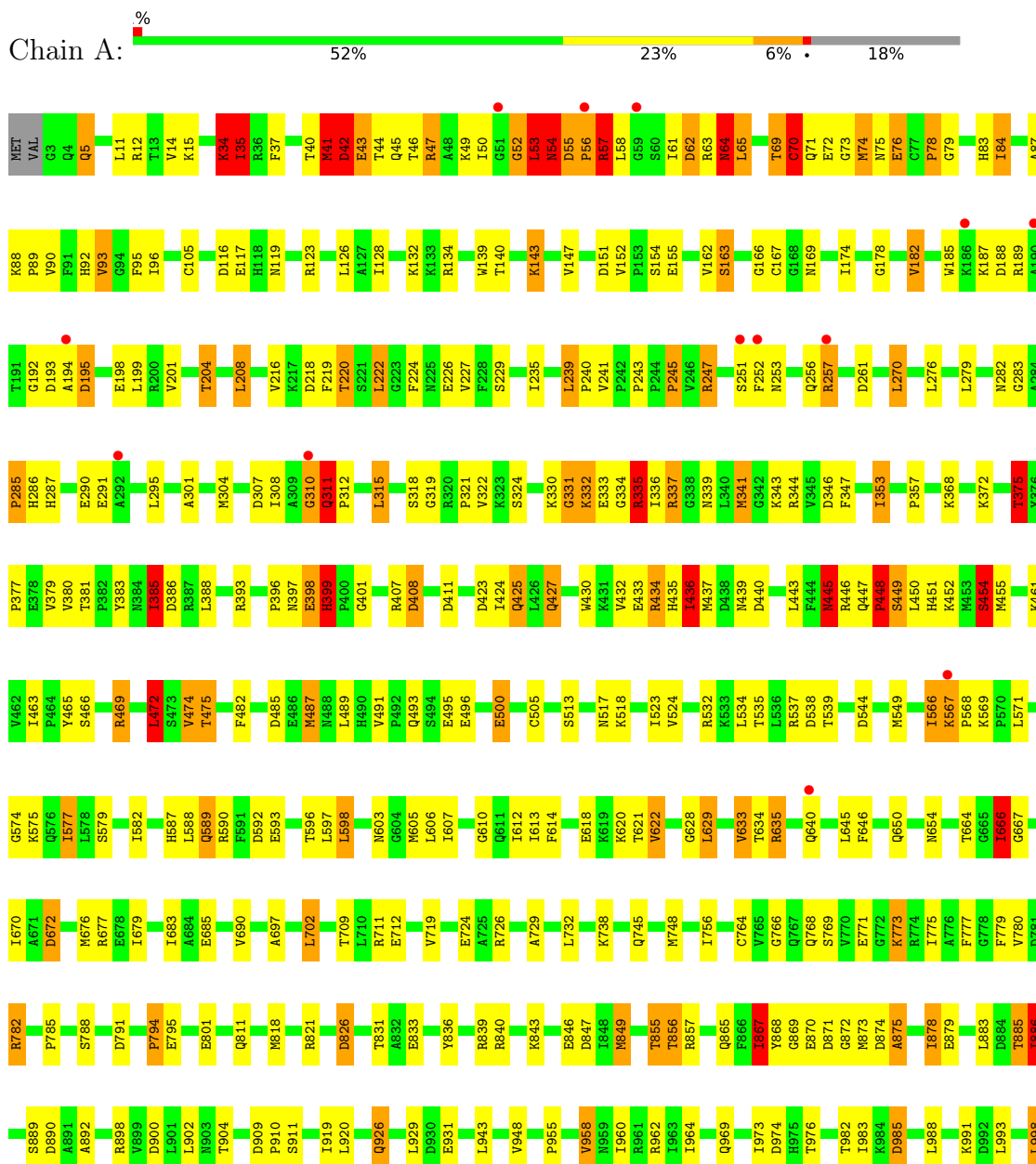


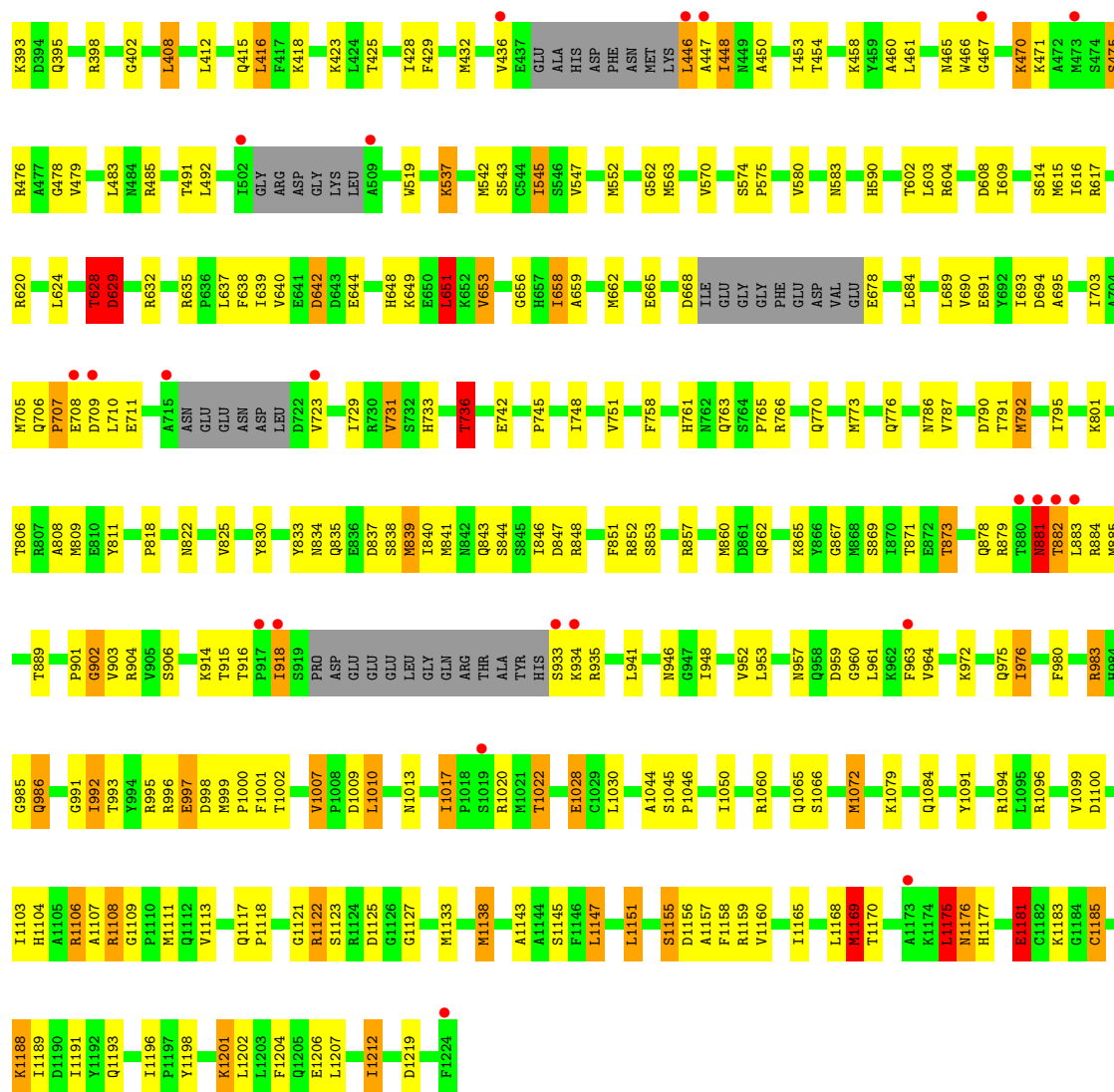
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	P	1	Total 31	C 11	N 5	O 12	P 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

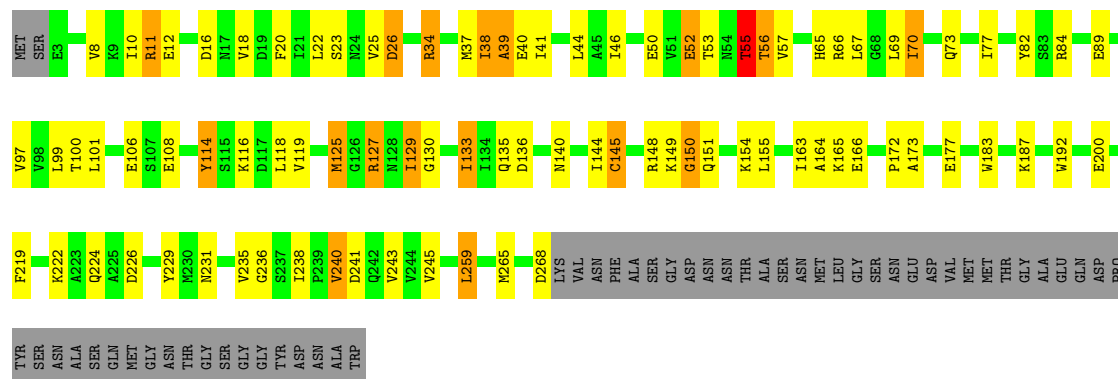
• Molecule 1: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB1



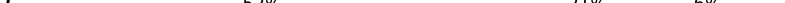


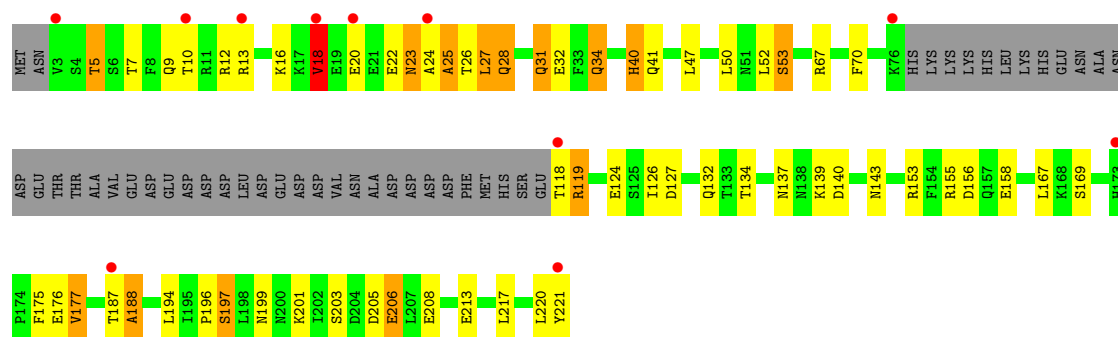
● Molecule 3: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB3

Chain C: 56% 22% 5% 16%

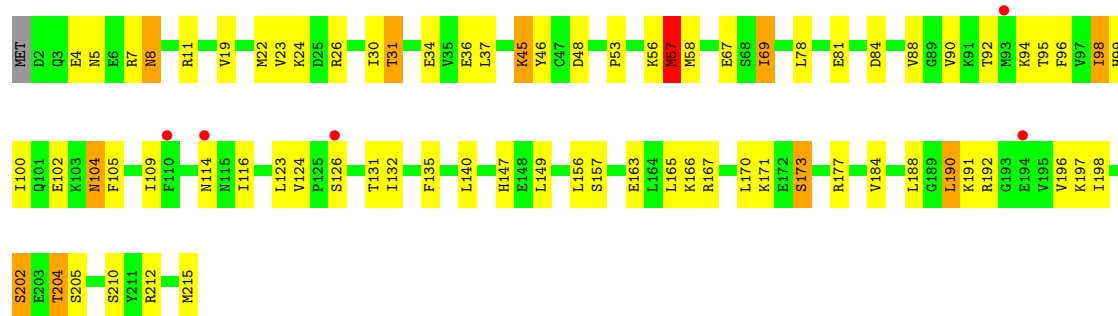


- Molecule 4: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB4

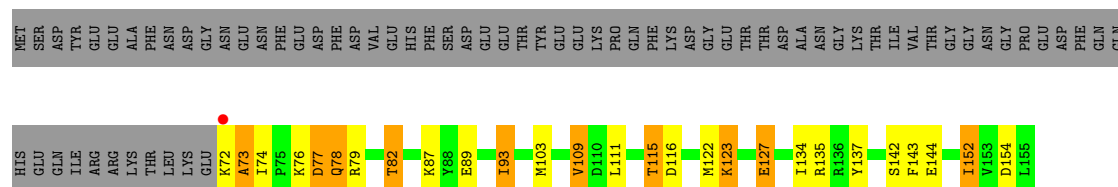
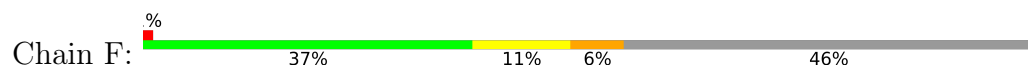
Chain D: 



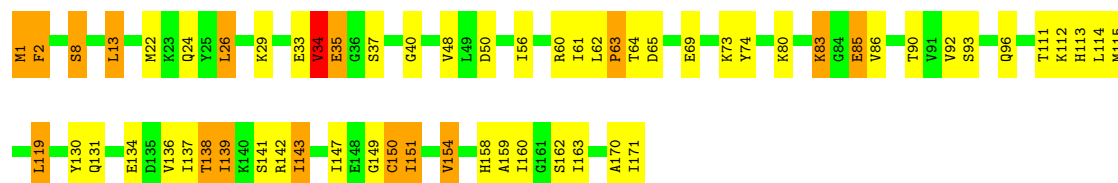
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2

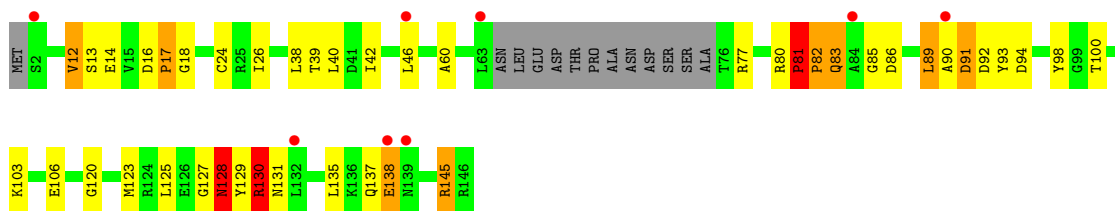


• Molecule 7: RPB7, DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB7

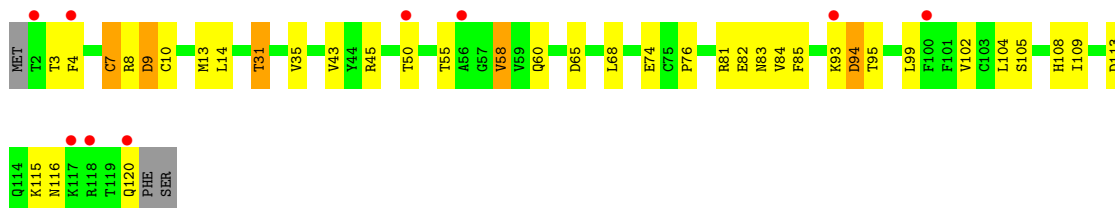


• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3





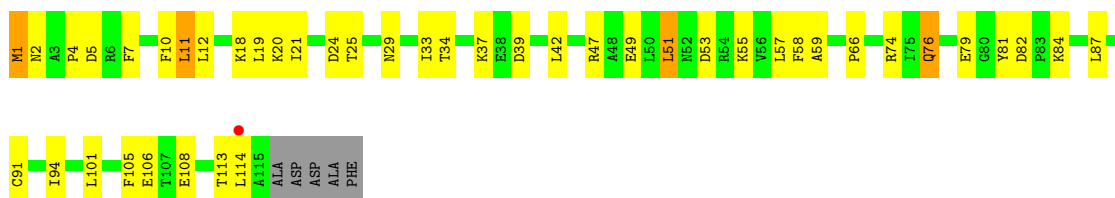
• Molecule 9: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB9



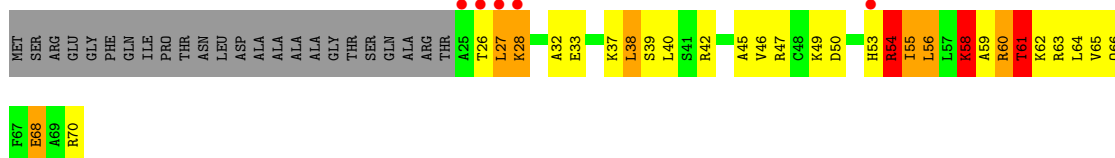
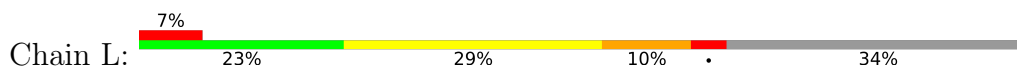
• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5



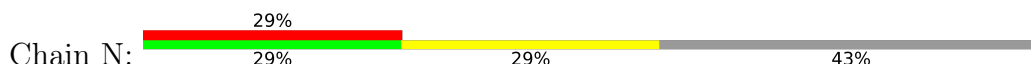
• Molecule 11: DNA-DIRECTED RNA POLYMERASE II SUBUNIT RPB11



• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4



• Molecule 13: NON TEMPLATE DNA 5'-D(*TP*AP*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*TP)-3'

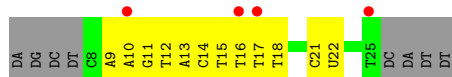
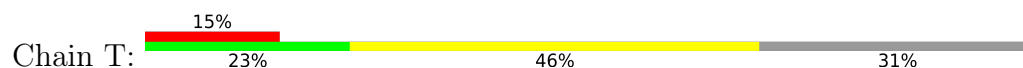




- Molecule 14: TRANSCRIPT RNA 5'-R(*CP*AP*GP*GP*AP)-3'



- Molecule 15: TEMPLATE DNA 5'-D(*AP*GP*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*TP*TP*TP*CP*CP*BRU*GP*GP*TP*CP*AP*TP*TP)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	223.68Å 394.17Å 283.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.61 – 3.40 54.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (54.61-3.40) 97.7 (54.61-3.40)	Depositor EDS
R_{merge}	0.63	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.40Å)	Xtriage
Refinement program	BUSTER 2.11.2	Depositor
R, R_{free}	0.160 , 0.188 0.181 , 0.206	Depositor DCC
R_{free} test set	3319 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	111.9	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 116.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.039 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31855	wwPDB-VP
Average B, all atoms (Å ²)	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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, ZN, MG, BRU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	12/11382 (0.1%)	1.56	151/15394 (1.0%)
2	B	0.87	1/9029 (0.0%)	1.48	94/12171 (0.8%)
3	C	0.87	0/2133	1.46	22/2891 (0.8%)
4	D	0.89	1/1444 (0.1%)	1.58	26/1935 (1.3%)
5	E	0.80	0/1788	1.44	21/2406 (0.9%)
6	F	0.98	0/691	1.47	7/933 (0.8%)
7	G	0.93	2/1368 (0.1%)	1.42	9/1844 (0.5%)
8	H	0.85	0/1086	1.42	17/1470 (1.2%)
9	I	0.83	0/989	1.38	9/1331 (0.7%)
10	J	0.90	0/541	1.57	5/727 (0.7%)
11	K	0.78	0/938	1.39	7/1267 (0.6%)
12	L	1.00	0/365	1.73	10/485 (2.1%)
13	N	0.59	0/184	0.65	0/282
14	P	0.74	0/101	0.66	0/156
15	T	0.66	0/383	0.75	0/586
All	All	0.89	16/32422 (0.0%)	1.49	378/43878 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	1	MET	C-N	7.68	1.44	1.33
1	A	57	ARG	CA-C	7.37	1.62	1.52
1	A	487	MET	SD-CE	-7.11	1.61	1.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	MET	SD-CE	6.97	1.97	1.79
7	G	1	MET	SD-CE	-6.95	1.62	1.79
1	A	867	ILE	CG1-CD1	6.80	1.78	1.51
1	A	1454	MET	CA-C	6.43	1.60	1.52
1	A	54	ASN	CA-C	6.10	1.60	1.52
1	A	56	PRO	C-N	5.88	1.42	1.33
4	D	18	VAL	CA-C	5.80	1.60	1.52
1	A	52	GLY	C-N	5.62	1.41	1.33
1	A	247	ARG	CA-C	5.38	1.59	1.53
1	A	57	ARG	C-N	5.37	1.41	1.33
1	A	69	THR	CA-CB	5.21	1.62	1.53
2	B	881	ASN	C-N	5.12	1.40	1.33
1	A	676	MET	SD-CE	5.11	1.92	1.79

All (378) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	39	ALA	N-CA-C	12.16	126.64	111.69
2	B	1155	SER	CA-C-N	10.72	135.01	120.54
2	B	1155	SER	C-N-CA	10.72	135.01	120.54
1	A	34	LYS	CA-C-N	10.29	140.22	121.70
1	A	34	LYS	C-N-CA	10.29	140.22	121.70
2	B	1156	ASP	N-CA-C	9.40	122.39	111.11
7	G	34	VAL	N-CA-C	9.33	119.87	110.82
10	J	5	VAL	N-CA-C	-9.13	97.81	109.58
8	H	81	PRO	N-CA-C	9.06	121.75	110.70
4	D	26	THR	N-CA-C	-8.86	102.03	112.92
1	A	1403	GLU	CA-C-N	-8.79	108.57	122.73
1	A	1403	GLU	C-N-CA	-8.79	108.57	122.73
1	A	72	GLU	N-CA-C	8.59	121.42	111.11
3	C	135	GLN	CA-C-N	8.50	132.89	120.90
3	C	135	GLN	C-N-CA	8.50	132.89	120.90
8	H	92	ASP	N-CA-C	-8.50	101.36	112.41
1	A	64	ASN	N-CA-C	-8.40	98.04	110.48
1	A	56	PRO	CA-C-N	8.21	137.23	121.54
1	A	56	PRO	C-N-CA	8.21	137.23	121.54
2	B	1122	ARG	CA-C-N	8.18	131.07	120.44
2	B	1122	ARG	C-N-CA	8.18	131.07	120.44
1	A	194	ALA	CA-C-N	8.09	136.26	121.70
1	A	194	ALA	C-N-CA	8.09	136.26	121.70
1	A	452	LYS	N-CA-C	-8.04	102.51	111.28
12	L	62	LYS	N-CA-C	-7.92	102.25	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	648	HIS	N-CA-C	7.88	119.96	110.19
1	A	219	PHE	CA-CB-CG	7.78	121.58	113.80
3	C	89	GLU	N-CA-C	-7.73	97.43	109.25
2	B	903	VAL	N-CA-C	7.72	119.42	109.30
1	A	143	LYS	CA-C-N	7.68	130.42	120.44
1	A	143	LYS	C-N-CA	7.68	130.42	120.44
12	L	55	ILE	N-CA-C	7.68	117.64	110.42
2	B	338	GLY	CA-C-N	7.66	135.48	121.70
2	B	338	GLY	C-N-CA	7.66	135.48	121.70
10	J	9	SER	N-CA-C	7.64	119.24	111.07
1	A	1419	ASP	CA-C-N	7.57	130.75	120.38
1	A	1419	ASP	C-N-CA	7.57	130.75	120.38
4	D	188	ALA	N-CA-C	-7.55	103.06	111.82
1	A	341	MET	CA-C-N	7.51	127.39	121.61
1	A	341	MET	C-N-CA	7.51	127.39	121.61
7	G	64	THR	N-CA-C	7.36	119.30	111.28
1	A	399	HIS	N-CA-CB	7.33	123.41	110.37
1	A	445	ASN	CA-CB-CG	7.29	119.89	112.60
2	B	1177	HIS	N-CA-C	-7.27	103.56	113.30
2	B	976	ILE	N-CA-C	7.25	117.38	110.42
1	A	485	ASP	CA-CB-CG	7.25	119.85	112.60
1	A	35	ILE	N-CA-CB	7.24	123.81	111.50
1	A	42	ASP	CA-CB-CG	7.24	119.84	112.60
4	D	31	GLN	N-CA-C	-7.23	103.47	111.36
11	K	2	ASN	CA-C-N	7.12	132.70	121.17
11	K	2	ASN	C-N-CA	7.12	132.70	121.17
1	A	218	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	537	ARG	CA-C-N	6.95	130.52	120.38
1	A	537	ARG	C-N-CA	6.95	130.52	120.38
1	A	439	ASN	CB-CA-C	6.93	116.69	109.83
2	B	628	THR	CA-C-N	6.93	134.77	121.54
2	B	628	THR	C-N-CA	6.93	134.77	121.54
2	B	902	GLY	CA-C-N	6.93	130.80	120.69
2	B	902	GLY	C-N-CA	6.93	130.80	120.69
2	B	102	VAL	N-CA-C	6.88	117.95	107.77
2	B	366	GLN	N-CA-C	-6.84	104.83	113.72
1	A	1403	GLU	N-CA-C	6.83	125.34	110.80
5	E	5	ASN	CA-C-N	6.81	129.71	120.38
5	E	5	ASN	C-N-CA	6.81	129.71	120.38
1	A	224	PHE	N-CA-C	6.80	118.78	110.41
1	A	54	ASN	CA-CB-CG	6.78	119.38	112.60
1	A	472	LEU	N-CA-C	6.78	119.50	111.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	296	GLU	N-CA-C	-6.76	103.37	111.69
4	D	53	SER	CA-C-N	6.73	129.54	120.65
4	D	53	SER	C-N-CA	6.73	129.54	120.65
1	A	466	SER	N-CA-C	6.73	120.95	113.21
3	C	82	TYR	N-CA-C	-6.73	99.57	110.20
1	A	1112	LYS	N-CA-C	6.71	118.39	111.14
1	A	874	ASP	CA-CB-CG	6.71	119.31	112.60
8	H	12	VAL	N-CA-C	6.70	117.09	108.12
2	B	1219	ASP	CA-CB-CG	6.68	119.28	112.60
12	L	58	LYS	N-CA-C	6.64	121.47	113.23
2	B	478	GLY	CA-C-N	6.63	128.92	120.56
2	B	478	GLY	C-N-CA	6.63	128.92	120.56
1	A	794	PRO	CA-C-N	6.62	129.16	120.28
1	A	794	PRO	C-N-CA	6.62	129.16	120.28
1	A	408	ASP	CA-CB-CG	6.62	119.22	112.60
1	A	73	GLY	CA-C-N	6.61	134.16	121.54
1	A	73	GLY	C-N-CA	6.61	134.16	121.54
2	B	629	ASP	CA-CB-CG	6.59	119.19	112.60
2	B	1185	CYS	N-CA-C	-6.59	104.62	114.64
1	A	396	PRO	N-CA-C	6.55	122.09	114.03
3	C	40	GLU	N-CA-C	6.51	122.12	112.94
3	C	183	TRP	N-CA-C	-6.49	98.65	108.96
1	A	998	LEU	N-CA-C	6.46	119.24	108.96
1	A	78	PRO	N-CA-C	-6.39	101.82	111.41
1	A	985	ASP	CA-CB-CG	6.37	118.97	112.60
1	A	34	LYS	N-CA-C	-6.37	97.90	108.34
1	A	229	SER	N-CA-C	6.36	117.82	107.32
9	I	9	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	1371	LEU	CA-C-N	6.34	128.54	120.56
1	A	1371	LEU	C-N-CA	6.34	128.54	120.56
1	A	1404	GLU	N-CA-C	6.32	119.92	112.72
5	E	173	SER	CA-C-N	6.32	130.80	120.63
5	E	173	SER	C-N-CA	6.32	130.80	120.63
1	A	677	ARG	CA-C-N	6.30	129.01	120.38
1	A	677	ARG	C-N-CA	6.30	129.01	120.38
3	C	38	ILE	CA-C-N	6.28	131.31	120.58
3	C	38	ILE	C-N-CA	6.28	131.31	120.58
12	L	60	ARG	N-CA-C	6.26	118.38	110.24
1	A	495	GLU	CA-C-N	6.26	128.95	120.44
1	A	495	GLU	C-N-CA	6.26	128.95	120.44
3	C	136	ASP	CA-CB-CG	6.23	118.83	112.60
2	B	1121	GLY	CA-C-N	6.20	128.87	120.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1121	GLY	C-N-CA	6.20	128.87	120.38
2	B	1013	ASN	N-CA-C	6.19	117.45	109.65
6	F	77	ASP	N-CA-C	-6.18	99.94	109.76
2	B	694	ASP	CA-CB-CG	6.18	118.78	112.60
9	I	93	LYS	CA-C-N	6.18	128.88	120.54
9	I	93	LYS	C-N-CA	6.18	128.88	120.54
4	D	132	GLN	N-CA-C	6.17	118.08	111.36
2	B	703	ILE	N-CA-C	6.16	117.46	108.53
1	A	1097	GLY	CA-C-N	6.08	126.27	120.43
1	A	1097	GLY	C-N-CA	6.08	126.27	120.43
2	B	1022	THR	CB-CA-C	6.08	120.07	111.74
1	A	539	THR	N-CA-C	6.07	118.08	108.67
1	A	47	ARG	CA-C-N	6.06	133.12	121.54
1	A	47	ARG	C-N-CA	6.06	133.12	121.54
1	A	398	GLU	CA-C-O	-6.05	114.10	121.36
4	D	18	VAL	CA-C-N	6.05	132.59	121.70
4	D	18	VAL	C-N-CA	6.05	132.59	121.70
2	B	45	SER	CA-C-N	6.03	128.64	120.38
2	B	45	SER	C-N-CA	6.03	128.64	120.38
1	A	408	ASP	CA-C-N	6.02	130.33	120.63
1	A	408	ASP	C-N-CA	6.02	130.33	120.63
2	B	188	ASP	CA-CB-CG	6.02	118.62	112.60
5	E	5	ASN	N-CA-C	-6.02	104.64	112.23
5	E	95	THR	CA-C-N	6.01	128.33	120.28
5	E	95	THR	C-N-CA	6.01	128.33	120.28
1	A	436	ILE	CB-CA-C	5.98	120.25	111.33
2	B	1169	MET	CA-C-N	5.98	128.57	120.38
2	B	1169	MET	C-N-CA	5.98	128.57	120.38
1	A	885	THR	CB-CA-C	5.96	120.63	110.74
11	K	53	ASP	CA-CB-CG	5.95	118.55	112.60
12	L	55	ILE	N-CA-CB	5.94	117.36	110.65
2	B	851	PHE	N-CA-C	5.93	120.32	113.38
9	I	116	ASN	N-CA-C	5.92	119.37	109.95
1	A	70	CYS	CA-C-N	-5.90	112.41	122.56
1	A	70	CYS	C-N-CA	-5.90	112.41	122.56
1	A	54	ASN	CA-C-N	5.90	136.20	121.80
1	A	54	ASN	C-N-CA	5.90	136.20	121.80
1	A	222	LEU	N-CA-C	-5.88	102.94	110.53
1	A	311	GLN	N-CA-C	5.88	122.81	109.81
8	H	137	GLN	CA-C-N	5.86	128.72	120.28
8	H	137	GLN	C-N-CA	5.86	128.72	120.28
8	H	131	ASN	CA-CB-CG	5.85	118.45	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	65	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	614	PHE	CA-CB-CG	5.83	119.63	113.80
5	E	96	PHE	CA-CB-CG	5.82	119.62	113.80
1	A	672	ASP	CA-CB-CG	5.82	118.42	112.60
2	B	881	ASN	CA-C-N	5.81	128.35	120.44
2	B	881	ASN	C-N-CA	5.81	128.35	120.44
1	A	535	THR	N-CA-C	5.81	120.00	113.02
3	C	145	CYS	N-CA-C	5.81	117.05	108.86
1	A	777	PHE	CA-CB-CG	5.78	119.58	113.80
1	A	5	GLN	N-CA-C	5.77	118.34	110.55
3	C	114	TYR	CA-C-N	5.77	128.28	120.38
3	C	114	TYR	C-N-CA	5.77	128.28	120.38
6	F	154	ASP	CA-CB-CG	5.76	118.36	112.60
1	A	875	ALA	N-CA-C	5.75	118.29	111.33
1	A	334	GLY	CA-C-N	5.75	132.52	121.54
1	A	334	GLY	C-N-CA	5.75	132.52	121.54
6	F	116	ASP	CA-CB-CG	5.73	118.33	112.60
1	A	69	THR	CA-C-N	5.72	132.47	121.54
1	A	69	THR	C-N-CA	5.72	132.47	121.54
2	B	998	ASP	CA-CB-CG	5.72	118.32	112.60
1	A	399	HIS	CA-CB-CG	-5.72	108.08	113.80
2	B	229	ALA	CA-C-N	5.72	128.13	120.58
2	B	229	ALA	C-N-CA	5.72	128.13	120.58
5	E	53	PRO	N-CA-C	5.72	120.21	110.95
1	A	123	ARG	CA-C-N	5.69	128.18	120.44
1	A	123	ARG	C-N-CA	5.69	128.18	120.44
2	B	733	HIS	CA-C-N	5.69	128.47	120.28
2	B	733	HIS	C-N-CA	5.69	128.47	120.28
2	B	707	PRO	CA-C-N	5.68	128.17	120.38
2	B	707	PRO	C-N-CA	5.68	128.17	120.38
1	A	898	ARG	N-CA-C	5.68	118.48	109.96
1	A	833	GLU	CA-C-N	5.66	128.43	120.28
1	A	833	GLU	C-N-CA	5.66	128.43	120.28
11	K	39	ASP	CA-CB-CG	5.66	118.26	112.60
4	D	24	ALA	CA-C-N	5.64	131.35	122.49
4	D	24	ALA	C-N-CA	5.64	131.35	122.49
5	E	171	LYS	N-CA-C	-5.64	100.98	109.95
2	B	276	ILE	CA-C-N	5.64	128.63	120.79
2	B	276	ILE	C-N-CA	5.64	128.63	120.79
2	B	465	ASN	CA-CB-CG	5.64	118.24	112.60
1	A	474	VAL	CA-C-N	5.64	128.15	120.54
1	A	474	VAL	C-N-CA	5.64	128.15	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	128	ASN	CA-C-N	5.64	130.26	120.68
8	H	128	ASN	C-N-CA	5.64	130.26	120.68
1	A	931	GLU	N-CA-C	-5.63	104.84	110.97
5	E	147	HIS	CA-C-N	5.63	128.14	120.54
5	E	147	HIS	C-N-CA	5.63	128.14	120.54
2	B	470	LYS	CA-C-N	5.62	130.51	122.08
2	B	470	LYS	C-N-CA	5.62	130.51	122.08
1	A	1416	ALA	CA-C-N	5.61	128.81	120.90
1	A	1416	ALA	C-N-CA	5.61	128.81	120.90
4	D	31	GLN	CA-C-N	5.60	127.72	120.44
4	D	31	GLN	C-N-CA	5.60	127.72	120.44
5	E	163	GLU	CB-CG-CD	5.60	122.12	112.60
12	L	49	LYS	CA-C-N	5.59	132.22	121.54
12	L	49	LYS	C-N-CA	5.59	132.22	121.54
2	B	906	SER	N-CA-C	5.57	122.66	110.80
1	A	900	ASP	CA-CB-CG	5.57	118.17	112.60
2	B	359	GLU	N-CA-C	5.56	120.05	112.04
2	B	791	THR	N-CA-C	-5.56	101.42	109.59
3	C	26	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	1341	ILE	N-CA-C	5.54	116.93	110.62
12	L	64	LEU	N-CA-C	5.53	118.94	110.20
12	L	61	THR	N-CA-C	5.53	117.42	110.24
1	A	1127	ASP	CA-CB-CG	5.52	118.12	112.60
2	B	642	ASP	CA-CB-CG	5.51	118.11	112.60
1	A	251	SER	N-CA-C	5.50	118.60	108.58
3	C	200	GLU	N-CA-C	5.49	118.03	111.71
4	D	25	ALA	CA-C-N	5.49	131.44	122.65
4	D	25	ALA	C-N-CA	5.49	131.44	122.65
3	C	55	THR	N-CA-C	-5.49	105.38	113.61
1	A	724	GLU	CA-C-N	5.47	127.56	120.44
1	A	724	GLU	C-N-CA	5.47	127.56	120.44
7	G	8	SER	N-CA-C	5.46	116.36	107.23
7	G	141	SER	N-CA-C	5.46	118.15	110.23
8	H	129	TYR	N-CA-C	5.46	119.11	112.23
2	B	339	THR	CA-C-N	5.45	131.96	121.54
2	B	339	THR	C-N-CA	5.45	131.96	121.54
2	B	825	VAL	N-CA-C	5.45	116.32	108.48
2	B	1028	GLU	CA-C-N	5.44	127.51	120.44
2	B	1028	GLU	C-N-CA	5.44	127.51	120.44
1	A	71	GLN	CA-C-N	5.43	127.88	120.54
1	A	71	GLN	C-N-CA	5.43	127.88	120.54
8	H	16	ASP	N-CA-C	5.43	120.68	109.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633	VAL	N-CA-CB	5.42	116.89	110.55
1	A	791	ASP	CA-CB-CG	5.42	118.02	112.60
2	B	294	ASP	CA-CB-CG	5.40	118.00	112.60
2	B	818	PRO	N-CA-C	5.40	118.78	111.22
7	G	40	GLY	CA-C-N	5.38	127.49	120.28
7	G	40	GLY	C-N-CA	5.38	127.49	120.28
1	A	331	GLY	CA-C-N	5.38	131.81	121.54
1	A	331	GLY	C-N-CA	5.38	131.81	121.54
2	B	343	ILE	CA-C-N	5.37	131.80	121.54
2	B	343	ILE	C-N-CA	5.37	131.80	121.54
9	I	31	THR	N-CA-C	-5.37	106.66	113.43
12	L	32	ALA	N-CA-C	5.37	117.89	111.71
2	B	648	HIS	CA-C-N	5.37	130.03	121.66
2	B	648	HIS	C-N-CA	5.37	130.03	121.66
2	B	320	ASP	CA-CB-CG	5.37	117.97	112.60
1	A	524	VAL	N-CA-CB	-5.36	105.01	112.52
1	A	436	ILE	CA-CB-CG2	5.36	119.61	110.50
2	B	340	ALA	CA-C-N	5.35	131.77	121.54
2	B	340	ALA	C-N-CA	5.35	131.77	121.54
1	A	666	ILE	N-CA-CB	5.35	119.80	110.65
2	B	885	MET	CA-C-N	5.35	128.69	120.82
2	B	885	MET	C-N-CA	5.35	128.69	120.82
5	E	57	MET	CA-C-N	5.33	127.74	120.54
5	E	57	MET	C-N-CA	5.33	127.74	120.54
11	K	106	GLU	CA-C-N	5.33	128.21	120.79
11	K	106	GLU	C-N-CA	5.33	128.21	120.79
2	B	736	THR	N-CA-C	-5.33	106.72	114.12
5	E	24	LYS	CA-C-N	5.32	127.67	120.38
5	E	24	LYS	C-N-CA	5.32	127.67	120.38
9	I	10	CYS	CA-C-N	5.32	131.70	121.54
9	I	10	CYS	C-N-CA	5.32	131.70	121.54
1	A	308	ILE	CA-C-N	5.32	127.72	120.54
1	A	308	ILE	C-N-CA	5.32	127.72	120.54
4	D	25	ALA	N-CA-C	-5.30	105.51	112.41
3	C	222	LYS	CA-C-N	5.30	128.63	121.05
3	C	222	LYS	C-N-CA	5.30	128.63	121.05
10	J	55	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	116	ASP	N-CA-C	5.29	115.01	108.19
5	E	126	SER	N-CA-C	5.27	117.77	111.71
10	J	26	GLN	CA-C-N	5.26	127.64	120.54
10	J	26	GLN	C-N-CA	5.26	127.64	120.54
4	D	52	LEU	CA-C-N	5.25	127.63	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	52	LEU	C-N-CA	5.25	127.63	120.54
1	A	1237	ILE	N-CA-C	5.25	116.28	108.46
2	B	454	THR	CA-C-N	5.24	127.61	120.54
2	B	454	THR	C-N-CA	5.24	127.61	120.54
1	A	310	GLY	CA-C-N	5.24	134.58	121.80
1	A	310	GLY	C-N-CA	5.24	134.58	121.80
1	A	818	MET	CA-C-N	5.24	125.75	119.94
1	A	818	MET	C-N-CA	5.24	125.75	119.94
4	D	143	ASN	CA-CB-CG	5.24	117.83	112.60
2	B	1158	PHE	CA-CB-CG	5.23	119.03	113.80
5	E	8	ASN	CA-C-N	5.23	127.10	120.72
5	E	8	ASN	C-N-CA	5.23	127.10	120.72
2	B	651	LEU	CA-C-N	5.23	128.66	120.82
2	B	651	LEU	C-N-CA	5.23	128.66	120.82
1	A	95	PHE	N-CA-C	5.22	119.50	113.18
6	F	87	LYS	CA-C-N	5.22	127.71	120.29
6	F	87	LYS	C-N-CA	5.22	127.71	120.29
1	A	592	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	1223	ASP	N-CA-C	-5.21	106.94	113.72
2	B	1001	PHE	N-CA-C	5.21	117.73	109.50
1	A	78	PRO	CA-C-N	-5.21	114.29	121.06
1	A	78	PRO	C-N-CA	-5.21	114.29	121.06
2	B	210	LYS	CA-C-N	5.21	129.82	123.10
2	B	210	LYS	C-N-CA	5.21	129.82	123.10
4	D	70	PHE	CA-CB-CG	5.20	119.00	113.80
1	A	285	PRO	CA-C-N	5.19	131.46	121.54
1	A	285	PRO	C-N-CA	5.19	131.46	121.54
2	B	1099	VAL	N-CA-C	5.19	115.63	110.23
1	A	375	THR	N-CA-CB	-5.18	102.22	111.08
2	B	809	MET	CA-C-N	5.18	127.17	120.44
2	B	809	MET	C-N-CA	5.18	127.17	120.44
1	A	411	ASP	CA-C-N	5.17	129.22	121.72
1	A	411	ASP	C-N-CA	5.17	129.22	121.72
3	C	34	ARG	CA-C-N	5.17	127.53	120.54
3	C	34	ARG	C-N-CA	5.17	127.53	120.54
4	D	24	ALA	N-CA-C	5.17	121.81	110.80
1	A	1234	GLU	N-CA-C	5.16	117.31	111.11
3	C	65	HIS	CA-C-N	5.16	127.15	120.44
3	C	65	HIS	C-N-CA	5.16	127.15	120.44
8	H	130	ARG	CA-C-N	5.16	127.47	120.65
8	H	130	ARG	C-N-CA	5.16	127.47	120.65
1	A	53	LEU	N-CA-CB	5.16	119.20	110.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	26	THR	CA-C-N	5.15	129.44	122.07
4	D	26	THR	C-N-CA	5.15	129.44	122.07
1	A	70	CYS	N-CA-C	-5.15	99.83	110.80
6	F	74	ILE	N-CA-C	5.15	114.57	108.96
4	D	140	ASP	CA-CB-CG	5.14	117.74	112.60
1	A	1436	ILE	N-CA-CB	-5.14	103.01	111.44
1	A	886	ILE	N-CA-C	5.14	120.02	109.34
8	H	86	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	425	GLN	CA-C-N	5.13	128.00	120.71
1	A	425	GLN	C-N-CA	5.13	128.00	120.71
4	D	124	GLU	CA-C-N	5.13	127.15	120.28
4	D	124	GLU	C-N-CA	5.13	127.15	120.28
1	A	495	GLU	N-CA-C	-5.13	105.77	112.23
5	E	48	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	454	SER	CA-C-N	5.12	129.87	122.44
1	A	454	SER	C-N-CA	5.12	129.87	122.44
1	A	892	ALA	CA-C-N	5.12	127.10	120.44
1	A	892	ALA	C-N-CA	5.12	127.10	120.44
8	H	85	GLY	CA-C-N	5.12	127.66	120.28
8	H	85	GLY	C-N-CA	5.12	127.66	120.28
1	A	883	LEU	CA-C-N	5.12	127.45	120.54
1	A	883	LEU	C-N-CA	5.12	127.45	120.54
2	B	881	ASN	CA-CB-CG	5.12	117.72	112.60
7	G	2	PHE	CA-CB-CG	5.12	118.92	113.80
1	A	116	ASP	CA-C-N	5.11	128.85	120.63
1	A	116	ASP	C-N-CA	5.11	128.85	120.63
1	A	826	ASP	CA-CB-CG	5.11	117.71	112.60
2	B	957	ASN	CA-CB-CG	5.10	117.70	112.60
6	F	82	THR	CB-CA-C	-5.10	101.46	109.52
9	I	58	VAL	CA-C-N	5.10	127.33	120.50
9	I	58	VAL	C-N-CA	5.10	127.33	120.50
1	A	245	PRO	CA-C-N	5.10	128.70	120.55
1	A	245	PRO	C-N-CA	5.10	128.70	120.55
1	A	1026	LEU	N-CA-C	5.09	118.98	112.26
2	B	475	SER	CA-C-N	5.09	131.26	121.54
2	B	475	SER	C-N-CA	5.09	131.26	121.54
1	A	92	HIS	N-CA-C	-5.09	101.67	109.76
2	B	1181	GLU	N-CA-C	5.08	121.63	110.80
1	A	1445	ILE	N-CA-CB	5.08	116.25	110.72
2	B	418	LYS	CA-C-N	5.06	127.06	120.28
2	B	418	LYS	C-N-CA	5.06	127.06	120.28
4	D	34	GLN	CB-CG-CD	-5.06	104.00	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	659	ALA	CA-C-N	5.06	127.06	120.28
2	B	659	ALA	C-N-CA	5.06	127.06	120.28
2	B	837	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	84	ILE	N-CA-CB	5.05	118.56	112.10
11	K	113	THR	CB-CA-C	5.05	119.31	112.09
1	A	890	ASP	CA-C-N	5.04	127.30	120.44
1	A	890	ASP	C-N-CA	5.04	127.30	120.44
8	H	145	ARG	CA-C-N	5.04	130.77	121.70
8	H	145	ARG	C-N-CA	5.04	130.77	121.70
2	B	69	LEU	CA-C-N	5.04	130.76	121.70
2	B	69	LEU	C-N-CA	5.04	130.76	121.70
1	A	1001	ARG	N-CA-C	5.03	120.41	113.97
1	A	119	ASN	CA-C-N	5.03	127.28	120.65
1	A	119	ASN	C-N-CA	5.03	127.28	120.65
2	B	1009	ASP	CA-CB-CG	5.02	117.62	112.60
7	G	50	ASP	CA-CB-CG	5.01	117.61	112.60
1	A	239	LEU	N-CA-C	5.00	116.65	109.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	LYS	Mainchain,Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11182	0	11244	223	0
2	B	8859	0	8901	165	0
3	C	2095	0	2051	44	0
4	D	1434	0	1460	16	0
5	E	1752	0	1776	32	0
6	F	679	0	701	18	0
7	G	1340	0	1357	34	0
8	H	1068	0	1040	13	0
9	I	971	0	927	10	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	532	0	542	19	0
11	K	920	0	929	24	0
12	L	363	0	386	14	0
13	N	165	0	92	5	0
14	P	90	0	44	1	0
15	T	365	0	204	14	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	C	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0
16	L	1	0	0	0	0
17	A	1	0	0	0	0
18	P	31	0	14	2	0
All	All	31855	0	31668	557	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 9.

All (557) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:ILE:CG1	1:A:867:ILE:CD1	1.78	1.60
4:D:40:HIS:HB3	7:G:73:LYS:HE3	1.26	1.13
1:A:53:LEU:HD23	1:A:54:ASN:H	1.22	1.01
5:E:4:GLU:HB3	5:E:7:ARG:HE	1.33	0.92
6:F:76:LYS:HA	6:F:79:ARG:HD3	1.55	0.89
1:A:1444:MET:HE1	6:F:135:ARG:HB2	1.57	0.85
7:G:1:MET:SD	7:G:2:PHE:N	2.48	0.85
1:A:847:ASP:HB3	1:A:1398:MET:HE1	1.59	0.85
1:A:61:ILE:HG22	1:A:62:ASP:H	1.41	0.84
12:L:28:LYS:HB2	12:L:39:SER:HA	1.60	0.83
1:A:53:LEU:HD23	1:A:54:ASN:N	1.93	0.81
1:A:63:ARG:HA	1:A:74:MET:HG3	1.62	0.80
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.44	0.79
3:C:56:THR:HG21	3:C:145:CYS:SG	2.22	0.79
1:A:53:LEU:CD2	1:A:54:ASN:H	1.94	0.79
1:A:683:ILE:HG21	1:A:801:GLU:HG3	1.64	0.79
1:A:902:LEU:HG	1:A:926:GLN:HG3	1.64	0.78
12:L:61:THR:HG21	12:L:63:ARG:HG2	1.64	0.78
2:B:999:MET:HG3	2:B:1000:PRO:HD2	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:48:ARG:O	10:J:52:THR:HG22	1.83	0.77
1:A:867:ILE:HD11	1:A:1000:LEU:HD21	1.66	0.77
2:B:563:MET:HE3	2:B:580:VAL:HB	1.67	0.76
7:G:1:MET:HE1	7:G:80:LYS:O	1.86	0.76
3:C:66:ARG:NH2	10:J:3:VAL:O	2.19	0.76
2:B:638:PHE:HB3	2:B:651:LEU:HD21	1.67	0.75
2:B:339:THR:HG21	2:B:351:TYR:HE2	1.53	0.74
6:F:77:ASP:O	6:F:78:GLN:HB2	1.88	0.73
1:A:41:MET:HB3	1:A:49:LYS:HA	1.71	0.73
1:A:855:THR:HG21	1:A:857:ARG:HE	1.51	0.73
4:D:203:SER:HB3	4:D:206:GLU:HB2	1.71	0.72
7:G:111:THR:HG22	7:G:113:HIS:H	1.53	0.72
1:A:347:PHE:HE1	1:A:375:THR:HG22	1.55	0.71
4:D:40:HIS:HB3	7:G:73:LYS:CE	2.16	0.71
11:K:21:ILE:HG12	11:K:33:ILE:HG12	1.72	0.71
1:A:34:LYS:HB3	1:A:83:HIS:CE1	2.25	0.71
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.31	0.70
1:A:869:GLY:O	5:E:204:THR:HG21	1.91	0.70
6:F:72:LYS:HE3	6:F:142:SER:HB3	1.72	0.69
2:B:839:MET:HE1	2:B:980:PHE:HB2	1.74	0.69
1:A:1079:MET:HE3	1:A:1359:ASP:HB2	1.73	0.69
1:A:93:VAL:HG22	1:A:301:ALA:HA	1.74	0.69
5:E:22:MET:HE2	5:E:26:ARG:HE	1.57	0.69
1:A:128:ILE:HB	1:A:134:ARG:HB2	1.73	0.69
9:I:7:CYS:HB2	9:I:14:LEU:HD21	1.76	0.68
15:T:16:DT:H3'	15:T:16:DT:C6	2.28	0.68
1:A:339:ASN:HB3	2:B:1117:GLN:NE2	2.10	0.67
2:B:344:LYS:HB3	2:B:347:LYS:HB2	1.76	0.67
1:A:855:THR:CG2	1:A:857:ARG:HE	2.07	0.67
1:A:726:ARG:HD3	1:A:766:GLY:HA3	1.76	0.67
11:K:7:PHE:HB2	11:K:11:LEU:HD22	1.75	0.67
2:B:583:ASN:HD21	2:B:628:THR:HG22	1.59	0.66
2:B:882:THR:HG1	2:B:935:ARG:N	1.94	0.66
15:T:16:DT:H3'	15:T:16:DT:H6	1.60	0.66
1:A:445:ASN:HB2	1:A:455:MET:HG2	1.77	0.66
2:B:172:ILE:HD13	2:B:178:ASN:HB3	1.77	0.66
2:B:1159:ARG:HD3	2:B:1193:GLN:HB2	1.76	0.66
13:N:4:DG:H1	15:T:14:DC:H42	1.43	0.66
2:B:996:ARG:HG3	2:B:1007:VAL:HG11	1.78	0.66
3:C:148:ARG:HD3	3:C:149:LYS:HG2	1.77	0.66
7:G:138:THR:HG22	7:G:139:ILE:H	1.60	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:58:PHE:HB3	11:K:76:GLN:HB3	1.77	0.66
4:D:176:GLU:OE2	4:D:197:SER:HB2	1.96	0.65
15:T:15:DT:H2'	15:T:16:DT:C2	2.30	0.65
10:J:1:MET:HG3	10:J:60:PHE:HE2	1.60	0.65
3:C:163:ILE:HD12	3:C:165:LYS:HB2	1.78	0.65
1:A:37:PHE:CD2	1:A:52:GLY:HA3	2.31	0.64
6:F:111:LEU:HD12	6:F:111:LEU:H	1.61	0.64
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.79	0.64
3:C:99:LEU:HD12	3:C:118:LEU:HB3	1.78	0.64
2:B:33:VAL:HG22	2:B:658:ILE:HD11	1.79	0.64
5:E:100:ILE:HG23	5:E:105:PHE:HB2	1.78	0.64
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.80	0.63
7:G:114:LEU:HD12	7:G:162:SER:HB2	1.80	0.63
1:A:62:ASP:HB3	1:A:64:ASN:O	1.98	0.63
1:A:283:GLY:O	1:A:285:PRO:HD3	1.99	0.63
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	1.80	0.63
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.81	0.63
1:A:383:TYR:HB3	6:F:115:THR:HG22	1.81	0.62
12:L:68:GLU:HB2	12:L:70:ARG:HD2	1.80	0.62
2:B:639:ILE:HD11	2:B:691:GLU:HB2	1.81	0.62
1:A:216:VAL:O	1:A:220:THR:HB	1.99	0.62
1:A:1444:MET:HG3	7:G:60:ARG:HA	1.82	0.62
1:A:37:PHE:HD2	1:A:52:GLY:HA3	1.64	0.62
1:A:40:THR:HG22	1:A:41:MET:HG2	1.81	0.62
1:A:140:THR:HA	1:A:143:LYS:HE2	1.83	0.61
1:A:368:LYS:HE2	1:A:399:HIS:HB2	1.81	0.61
13:N:5:DT:H2''	13:N:6:DA:C8	2.35	0.61
1:A:105:CYS:SG	1:A:139:TRP:HA	2.41	0.61
2:B:446:LEU:HD12	2:B:448:ILE:HD11	1.82	0.61
4:D:40:HIS:CB	7:G:73:LYS:HE3	2.18	0.61
7:G:35:GLU:HG3	7:G:48:VAL:HG23	1.83	0.60
2:B:865:LYS:HB2	2:B:961:LEU:HD21	1.83	0.60
3:C:241:ASP:O	3:C:245:VAL:HG23	2.00	0.60
2:B:339:THR:HG21	2:B:351:TYR:CE2	2.36	0.60
3:C:10:ILE:HD12	11:K:108:GLU:HB3	1.83	0.60
15:T:17:DT:H5'	15:T:18:DT:OP1	2.01	0.60
2:B:952:VAL:HB	12:L:58:LYS:HB2	1.83	0.60
1:A:870:GLU:HB2	5:E:204:THR:HG21	1.82	0.60
7:G:119:LEU:HD23	7:G:130:TYR:HB3	1.82	0.60
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.83	0.59
2:B:822:ASN:O	10:J:48:ARG:NH1	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.83	0.59
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.82	0.59
1:A:629:LEU:O	1:A:633:VAL:HG23	2.03	0.59
4:D:23:ASN:HA	4:D:28:GLN:O	2.02	0.59
11:K:57:LEU:HB2	11:K:76:GLN:HG2	1.84	0.59
2:B:918:ILE:HD13	2:B:935:ARG:HH12	1.67	0.59
5:E:94:LYS:HE2	5:E:98:ILE:HD11	1.85	0.59
3:C:55:THR:HB	3:C:151:GLN:HA	1.85	0.59
1:A:1101:LEU:HB2	1:A:1355:VAL:HG11	1.83	0.59
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.85	0.59
2:B:361:LEU:HD11	2:B:381:MET:HE1	1.85	0.58
2:B:882:THR:HG21	2:B:935:ARG:HA	1.84	0.58
7:G:83:LYS:HD2	7:G:149:GLY:HA2	1.85	0.58
1:A:871:ASP:HB3	5:E:204:THR:HG23	1.86	0.58
4:D:176:GLU:OE2	4:D:201:LYS:HE2	2.03	0.58
1:A:335:ARG:HD2	2:B:1206:GLU:OE1	2.04	0.58
3:C:97:VAL:HG21	3:C:129:ILE:HG23	1.85	0.57
2:B:653:VAL:HG22	2:B:689:LEU:HB3	1.84	0.57
2:B:801:LYS:O	10:J:52:THR:OG1	2.22	0.57
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.86	0.57
2:B:1109:GLY:O	2:B:1111:MET:HE2	2.05	0.57
1:A:41:MET:CB	1:A:49:LYS:HA	2.35	0.57
1:A:982:THR:HB	1:A:985:ASP:H	1.69	0.57
2:B:338:GLY:HA3	2:B:340:ALA:H	1.70	0.57
7:G:8:SER:HB3	7:G:73:LYS:HD2	1.85	0.57
7:G:1:MET:CE	7:G:80:LYS:O	2.52	0.57
2:B:1100:ASP:OD2	11:K:1:MET:HB3	2.05	0.56
15:T:16:DT:C6	15:T:16:DT:C3'	2.88	0.56
1:A:239:LEU:HD12	1:A:240:PRO:HD2	1.88	0.56
2:B:843:GLN:HA	2:B:846:ILE:HD12	1.86	0.56
4:D:18:VAL:HG22	4:D:20:GLU:H	1.70	0.56
1:A:347:PHE:H	2:B:1107:ALA:HA	1.71	0.56
1:A:448:PRO:O	1:A:449:SER:HB2	2.06	0.56
1:A:590:ARG:NH2	1:A:621:THR:OG1	2.38	0.56
2:B:629:ASP:HB3	2:B:632:ARG:HE	1.70	0.56
3:C:187:LYS:HG3	3:C:219:PHE:CE1	2.41	0.56
2:B:428:ILE:HG22	2:B:432:MET:HE2	1.88	0.55
7:G:26:LEU:HD13	7:G:56:ILE:HD11	1.87	0.55
10:J:2:ILE:HD12	10:J:57:ILE:HD13	1.87	0.55
11:K:1:MET:O	11:K:1:MET:HG2	2.06	0.55
4:D:167:LEU:HB3	4:D:177:VAL:HG22	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:983:ARG:HD2	2:B:1091:TYR:HB3	1.89	0.55
1:A:341:MET:HE2	1:A:843:LYS:HZ1	1.71	0.55
2:B:904:ARG:HG3	2:B:948:ILE:HG13	1.87	0.55
2:B:916:THR:O	2:B:935:ARG:HG2	2.07	0.55
2:B:34:ILE:HG12	2:B:542:MET:HE2	1.87	0.55
1:A:534:LEU:O	1:A:574:GLY:HA3	2.05	0.55
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.40	0.55
8:H:100:THR:HG23	8:H:138:GLU:HA	1.89	0.55
1:A:319:GLY:HA3	2:B:471:LYS:HG3	1.89	0.54
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	2.08	0.54
3:C:259:LEU:CD2	11:K:91:CYS:HB3	2.37	0.54
5:E:31:THR:HG23	5:E:34:GLU:HB2	1.88	0.54
2:B:425:THR:HA	2:B:428:ILE:HD12	1.88	0.54
5:E:90:VAL:HG23	5:E:123:LEU:HD11	1.89	0.54
2:B:216:GLU:OE1	2:B:537:LYS:HD2	2.08	0.54
2:B:882:THR:CG2	2:B:935:ARG:HA	2.37	0.54
1:A:341:MET:HE2	1:A:843:LYS:NZ	2.22	0.54
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.56	0.54
9:I:65:ASP:HB3	9:I:68:LEU:HD12	1.89	0.54
1:A:1172:LEU:C	1:A:1174:PHE:H	2.16	0.54
1:A:1074:GLU:HB3	1:A:1075:PRO:HD3	1.90	0.53
2:B:166:PHE:HZ	2:B:169:ARG:HG2	1.73	0.53
3:C:52:GLU:HB3	3:C:154:LYS:HB3	1.90	0.53
2:B:274:PRO:HG2	2:B:359:GLU:HB3	1.89	0.53
3:C:50:GLU:HG2	12:L:66:GLN:HG3	1.91	0.53
7:G:34:VAL:O	7:G:37:SER:HB3	2.08	0.53
8:H:89:LEU:C	8:H:91:ASP:H	2.16	0.53
1:A:567:LYS:HA	1:A:568:PRO:C	2.33	0.53
1:A:873:MET:HB3	1:A:878:ILE:HD11	1.90	0.53
2:B:34:ILE:HG12	2:B:542:MET:CE	2.38	0.53
5:E:135:PHE:HB3	5:E:140:LEU:HD11	1.91	0.53
1:A:315:LEU:HA	1:A:321:PRO:HA	1.90	0.53
1:A:446:ARG:HH22	18:P:1011:APC:HI'	1.73	0.53
1:A:187:LYS:HE3	1:A:198:GLU:HB2	1.91	0.53
1:A:1079:MET:HE2	1:A:1097:GLY:HA2	1.91	0.53
8:H:125:LEU:HG	8:H:130:ARG:HH22	1.73	0.53
1:A:566:ILE:HD11	8:H:98:TYR:HB2	1.91	0.52
2:B:67:SER:HB2	2:B:92:PHE:CD1	2.44	0.52
2:B:992:ILE:HD11	11:K:66:PRO:HB2	1.91	0.52
2:B:902:GLY:O	12:L:65:VAL:HG11	2.09	0.52
4:D:25:ALA:HB1	4:D:196:PRO:HG2	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:82:ASP:OD2	11:K:84:LYS:HB2	2.08	0.52
12:L:47:ARG:HH21	12:L:54:ARG:HE	1.58	0.52
5:E:22:MET:HE2	5:E:26:ARG:NE	2.24	0.52
7:G:85:GLU:HB3	7:G:147:ILE:HD12	1.91	0.52
1:A:1100:ARG:HH21	1:A:1351:GLU:HG2	1.73	0.52
7:G:142:ARG:HG2	7:G:171:ILE:HD12	1.91	0.52
2:B:238:ALA:HB3	2:B:256:VAL:HB	1.91	0.52
7:G:1:MET:HE1	7:G:80:LYS:C	2.34	0.52
1:A:40:THR:HB	1:A:257:ARG:CZ	2.40	0.52
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	1.92	0.52
2:B:776:GLN:HA	2:B:1096:ARG:HH11	1.74	0.52
8:H:127:GLY:N	8:H:130:ARG:HH21	2.08	0.52
2:B:1147:LEU:HD22	2:B:1151:LEU:HD22	1.92	0.52
1:A:35:ILE:HG22	1:A:84:ILE:CG2	2.40	0.51
2:B:839:MET:HE3	2:B:1010:LEU:HD21	1.92	0.51
1:A:353:ILE:HD12	1:A:482:PHE:CD1	2.46	0.51
2:B:1106:ARG:NH2	2:B:1118:PRO:HB3	2.25	0.51
1:A:399:HIS:O	1:A:401:GLY:N	2.43	0.51
1:A:1259:MET:HA	1:A:1262:LYS:HD2	1.92	0.51
2:B:121:ASN:HA	2:B:207:GLY:HA3	1.93	0.51
2:B:114:PRO:HG3	2:B:181:LEU:HD11	1.93	0.51
12:L:61:THR:CG2	12:L:63:ARG:HG2	2.39	0.51
5:E:124:VAL:HG13	5:E:132:ILE:HB	1.93	0.51
2:B:382:ILE:O	2:B:386:LEU:HG	2.11	0.51
3:C:265:MET:HE1	11:K:19:LEU:HB2	1.93	0.51
8:H:40:LEU:HD13	8:H:123:MET:HG3	1.93	0.51
1:A:588:LEU:HD23	1:A:607:ILE:HD12	1.92	0.51
1:A:667:GLY:HA2	1:A:670:ILE:HD12	1.93	0.50
3:C:259:LEU:HD22	11:K:91:CYS:HB3	1.92	0.50
2:B:206:ASN:HD21	2:B:458:LYS:HD3	1.76	0.50
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.93	0.50
3:C:46:ILE:HD13	3:C:67:LEU:O	2.10	0.50
10:J:9:SER:OG	10:J:48:ARG:NH2	2.43	0.50
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.47	0.50
6:F:79:ARG:HG2	6:F:144:GLU:HB3	1.93	0.50
1:A:1370:LEU:O	1:A:1374:VAL:HG23	2.10	0.50
1:A:1118:VAL:HG23	1:A:1306:LEU:HB2	1.93	0.50
2:B:865:LYS:HE2	2:B:869:SER:HA	1.94	0.50
3:C:116:LYS:HD3	3:C:140:ASN:HA	1.93	0.50
1:A:55:ASP:CG	1:A:55:ASP:O	2.54	0.50
1:A:42:ASP:O	1:A:44:THR:N	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:ILE:HD12	1:A:482:PHE:HD1	1.77	0.49
1:A:1376:THR:HG23	5:E:212:ARG:HH22	1.76	0.49
1:A:523:ILE:HD13	1:A:622:VAL:HG22	1.95	0.49
6:F:109:VAL:HG22	6:F:127:GLU:OE2	2.12	0.49
1:A:500:GLU:HG2	2:B:1143:ALA:HA	1.95	0.49
2:B:706:GLN:H	2:B:710:LEU:HD12	1.76	0.49
9:I:82:GLU:HB3	9:I:104:LEU:HB2	1.95	0.49
2:B:242:SER:OG	2:B:362:PRO:HD2	2.13	0.49
2:B:128:LEU:HD21	2:B:170:LEU:HB2	1.93	0.49
11:K:10:PHE:HD2	11:K:11:LEU:HD13	1.77	0.49
11:K:49:GLU:HG3	11:K:94:ILE:HG13	1.94	0.49
1:A:433:GLU:OE1	2:B:1108:ARG:NH2	2.46	0.49
1:A:849:MET:HE1	1:A:1440:ALA:HB1	1.94	0.49
1:A:870:GLU:HB2	5:E:204:THR:CG2	2.43	0.49
1:A:1077:THR:HG22	1:A:1081:LEU:HD12	1.94	0.49
2:B:976:ILE:HD11	2:B:992:ILE:HA	1.94	0.49
3:C:44:LEU:HB2	3:C:77:ILE:HD13	1.95	0.49
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.94	0.49
2:B:995:ARG:HB3	2:B:997:GLU:OE2	2.13	0.49
1:A:377:PRO:HD3	1:A:493:GLN:OE1	2.13	0.48
1:A:43:GLU:HB2	1:A:46:THR:HB	1.95	0.48
1:A:93:VAL:HG23	1:A:304:MET:HE3	1.95	0.48
2:B:603:LEU:HD22	2:B:608:ASP:HB2	1.94	0.48
5:E:165:LEU:HD23	5:E:170:LEU:HB2	1.95	0.48
2:B:311:LEU:HB3	9:I:4:PHE:HE1	1.78	0.48
3:C:149:LYS:HG3	3:C:150:GLY:H	1.79	0.48
1:A:346:ASP:HB3	2:B:1108:ARG:H	1.78	0.48
1:A:469:ARG:NH2	2:B:991:GLY:O	2.44	0.48
1:A:646:PHE:O	1:A:650:GLN:HG2	2.13	0.48
2:B:466:TRP:HB2	2:B:479:VAL:HG21	1.94	0.48
2:B:1169:MET:HE1	2:B:1201:LYS:HA	1.95	0.48
2:B:1175:LEU:O	2:B:1176:ASN:HB2	2.14	0.48
1:A:1036:ARG:HH11	1:A:1036:ARG:HG2	1.79	0.48
2:B:986:GLN:NE2	2:B:1022:THR:HG21	2.28	0.48
12:L:27:LEU:HD13	12:L:37:LYS:HG2	1.95	0.48
1:A:343:LYS:HD2	2:B:1151:LEU:HD12	1.95	0.48
1:A:347:PHE:CE1	1:A:375:THR:HG22	2.43	0.48
1:A:709:THR:HB	1:A:712:GLU:H	1.78	0.48
1:A:709:THR:HG23	9:I:94:ASP:HA	1.95	0.48
2:B:773:MET:HE2	2:B:985:GLY:HA2	1.95	0.48
7:G:131:GLN:HG2	7:G:136:VAL:HG22	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:HA3	1:A:243:PRO:CG	2.44	0.48
1:A:335:ARG:NH1	2:B:1206:GLU:OE2	2.46	0.48
2:B:483:LEU:HD11	2:B:491:THR:HG23	1.95	0.48
2:B:705:MET:HE2	2:B:745:PRO:HB3	1.96	0.48
1:A:87:ALA:HB3	1:A:276:LEU:HD23	1.96	0.48
1:A:579:SER:HA	1:A:582:ILE:HD12	1.96	0.48
13:N:8:DT:H3	15:T:10:DA:H61	1.61	0.48
1:A:993:LEU:HD22	1:A:1046:LEU:HD22	1.95	0.48
2:B:562:GLY:O	2:B:590:HIS:ND1	2.47	0.48
8:H:93:TYR:HA	8:H:145:ARG:HB3	1.96	0.48
1:A:886:ILE:HG12	1:A:943:LEU:HB3	1.95	0.47
1:A:878:ILE:CG2	1:A:955:PRO:HB2	2.44	0.47
1:A:1155:ASP:HB3	1:A:1241:ARG:HH21	1.79	0.47
1:A:1349:TYR:HA	1:A:1372:VAL:HG21	1.95	0.47
2:B:249:ARG:HH12	2:B:415:GLN:HA	1.80	0.47
11:K:55:LYS:HB3	11:K:81:TYR:CD2	2.49	0.47
1:A:62:ASP:C	1:A:64:ASN:H	2.22	0.47
1:A:836:TYR:CE1	1:A:840:ARG:HD2	2.49	0.47
2:B:770:GLN:HG2	2:B:983:ARG:C	2.39	0.47
2:B:1165:ILE:HD12	2:B:1185:CYS:HB3	1.97	0.47
1:A:1159:ARG:HG2	1:A:1174:PHE:HE2	1.79	0.47
2:B:901:PRO:HD2	12:L:60:ARG:HA	1.96	0.47
1:A:633:VAL:HG21	1:A:645:LEU:HD22	1.96	0.47
1:A:635:ARG:HH11	1:A:635:ARG:HA	1.80	0.47
2:B:684:LEU:HA	2:B:689:LEU:HD12	1.95	0.47
2:B:841:MET:O	2:B:993:THR:HA	2.15	0.47
3:C:163:ILE:CD1	3:C:165:LYS:HB2	2.42	0.47
5:E:19:VAL:O	5:E:23:VAL:HG23	2.15	0.47
10:J:7:CYS:HA	10:J:49:MET:HE3	1.95	0.47
1:A:151:ASP:HA	1:A:163:SER:HA	1.96	0.47
1:A:332:LYS:HB2	1:A:337:ARG:NH2	2.29	0.47
2:B:873:THR:O	2:B:914:LYS:HA	2.15	0.47
1:A:582:ILE:HG22	1:A:610:GLY:HA2	1.96	0.47
1:A:650:GLN:O	1:A:654:ASN:HB2	2.16	0.47
1:A:745:GLN:HA	1:A:748:MET:HE3	1.97	0.47
10:J:48:ARG:HE	10:J:49:MET:CE	2.28	0.47
11:K:10:PHE:CD2	11:K:11:LEU:HD13	2.50	0.47
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.97	0.46
2:B:310:MET:HE2	2:B:386:LEU:HB2	1.97	0.46
1:A:1152:ILE:HG12	1:A:1260:LEU:HD23	1.97	0.46
1:A:1442:ASP:HB2	6:F:137:TYR:HE2	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:46:TYR:CE1	5:E:58:MET:HA	2.51	0.46
5:E:198:ILE:HD13	5:E:212:ARG:HG3	1.97	0.46
1:A:243:PRO:HB2	1:A:245:PRO:HD2	1.98	0.46
2:B:467:GLY:HA3	2:B:475:SER:HB3	1.97	0.46
2:B:563:MET:CE	2:B:580:VAL:HB	2.42	0.46
11:K:24:ASP:OD2	11:K:74:ARG:NH1	2.48	0.46
1:A:388:LEU:HD13	1:A:432:VAL:HB	1.98	0.46
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.97	0.46
1:A:589:GLN:HG2	1:A:606:LEU:HD13	1.96	0.46
1:A:867:ILE:CD1	1:A:867:ILE:CB	2.80	0.46
1:A:1348:LEU:O	1:A:1352:VAL:HG23	2.16	0.46
3:C:37:MET:HA	3:C:41:ILE:HD12	1.98	0.46
2:B:131:ASP:HA	2:B:164:LYS:HB3	1.96	0.46
2:B:1002:THR:HG22	2:B:1072:MET:HE2	1.97	0.46
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.14	0.46
3:C:133:ILE:HG21	3:C:236:GLY:HA3	1.97	0.46
5:E:167:ARG:HA	5:E:167:ARG:HD3	1.69	0.46
12:L:60:ARG:HH22	12:L:65:VAL:HG22	1.81	0.46
1:A:182:VAL:HB	1:A:201:VAL:HG23	1.96	0.46
1:A:697:ALA:HB2	1:A:702:LEU:HD13	1.98	0.46
1:A:1335:ILE:HG23	1:A:1339:LEU:HD12	1.98	0.46
1:A:1435:PRO:HA	1:A:1439:GLY:O	2.16	0.46
4:D:27:LEU:HD22	4:D:27:LEU:HA	1.86	0.46
2:B:408:LEU:HD21	2:B:545:ILE:HD13	1.97	0.46
2:B:862:GLN:HB3	2:B:963:PHE:HD1	1.81	0.46
2:B:635:ARG:NH1	2:B:742:GLU:OE2	2.49	0.46
6:F:77:ASP:O	6:F:78:GLN:CB	2.61	0.46
10:J:48:ARG:O	10:J:52:THR:CG2	2.61	0.46
1:A:14:VAL:HB	1:A:1430:LEU:HD13	1.98	0.46
1:A:50:ILE:HG23	1:A:52:GLY:H	1.81	0.46
1:A:587:HIS:HB2	1:A:969:GLN:HE22	1.81	0.45
1:A:1155:ASP:HB3	1:A:1241:ARG:NH2	2.32	0.45
1:A:1426:GLU:H	1:A:1426:GLU:HG2	1.51	0.45
1:A:1318:THR:HB	5:E:11:ARG:HH12	1.81	0.45
2:B:839:MET:CE	2:B:980:PHE:HB2	2.43	0.45
6:F:76:LYS:HA	6:F:79:ARG:CD	2.37	0.45
1:A:79:GLY:HA3	1:A:243:PRO:HG3	1.98	0.45
1:A:449:SER:HA	1:A:454:SER:HB3	1.98	0.45
2:B:519:TRP:HZ2	2:B:705:MET:HE1	1.81	0.45
1:A:549:MET:HB3	1:A:577:ILE:HD13	1.98	0.45
3:C:125:MET:HB2	3:C:127:ARG:NE	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:188:LEU:HB2	5:E:190:LEU:HD23	1.99	0.45
1:A:780:VAL:O	1:A:782:ARG:HD3	2.16	0.45
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.80	0.45
1:A:1338:VAL:HG12	1:A:1339:LEU:HG	1.97	0.45
2:B:649:LYS:HD3	2:B:736:THR:O	2.16	0.45
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.52	0.45
1:A:427:GLN:HB2	1:A:430:TRP:CE2	2.52	0.45
1:A:771:GLU:O	1:A:773:LYS:HE2	2.16	0.45
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.99	0.45
2:B:1169:MET:CE	2:B:1204:PHE:HB2	2.47	0.45
2:B:1198:TYR:CE1	2:B:1201:LYS:HE3	2.52	0.45
5:E:88:VAL:HB	5:E:116:ILE:HG12	1.99	0.45
1:A:56:PRO:O	1:A:57:ARG:HG3	2.17	0.45
3:C:39:ALA:HA	3:C:164:ALA:HB3	1.98	0.45
3:C:173:ALA:HB2	3:C:243:VAL:HG11	1.98	0.45
1:A:353:ILE:HG21	1:A:487:MET:HE3	1.99	0.44
18:P:1011:APC:HN62	15:T:18:DT:H3	1.65	0.44
1:A:1193:LEU:HB3	1:A:1240:CYS:HB2	1.98	0.44
3:C:8:VAL:HG11	11:K:105:PHE:HD1	1.82	0.44
3:C:34:ARG:O	3:C:38:ILE:HD12	2.17	0.44
8:H:82:PRO:HB2	8:H:83:GLN:H	1.65	0.44
1:A:575:LYS:HD2	8:H:120:GLY:HA3	2.00	0.44
1:A:868:TYR:HD2	1:A:1058:VAL:HG21	1.81	0.44
2:B:852:ARG:HH22	12:L:70:ARG:C	2.26	0.44
14:P:8:G:H1	15:T:21:DC:H42	1.65	0.44
1:A:596:THR:HG22	1:A:598:LEU:H	1.82	0.44
1:A:1116:LEU:HB3	1:A:1308:THR:OG1	2.18	0.44
1:A:1293:SER:HB2	1:A:1294:PRO:HD2	1.99	0.44
9:I:102:VAL:HG22	9:I:109:ILE:HG13	1.99	0.44
15:T:14:DC:H2'	15:T:15:DT:C6	2.51	0.44
1:A:84:ILE:HG13	1:A:239:LEU:HB3	1.99	0.44
2:B:745:PRO:O	2:B:748:ILE:HG12	2.17	0.44
2:B:1100:ASP:HA	2:B:1103:ILE:HG22	2.00	0.44
6:F:93:ILE:HD11	6:F:134:ILE:HD11	1.98	0.44
1:A:5:GLN:O	2:B:1159:ARG:NH2	2.49	0.44
2:B:223:VAL:HG23	2:B:240:ILE:HD12	1.99	0.44
4:D:194:LEU:HD22	7:G:86:VAL:HG11	2.00	0.44
7:G:143:ILE:HG13	7:G:170:ALA:HA	2.00	0.44
1:A:709:THR:HG22	1:A:711:ARG:H	1.82	0.44
2:B:35:SER:HA	2:B:811:TYR:CE1	2.53	0.44
2:B:848:ARG:HA	3:C:69:LEU:HD21	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:MET:CE	1:A:612:ILE:HG23	2.48	0.44
1:A:958:VAL:HG22	1:A:1052:GLN:HB3	1.99	0.44
1:A:1433:MET:HE3	7:G:63:PRO:HB3	1.99	0.44
7:G:137:ILE:HG12	7:G:143:ILE:HD11	1.99	0.44
8:H:17:PRO:HB3	8:H:24:CYS:SG	2.57	0.44
1:A:50:ILE:C	1:A:52:GLY:H	2.26	0.44
1:A:93:VAL:CG2	1:A:301:ALA:HA	2.46	0.44
1:A:1151:GLU:HG2	9:I:45:ARG:HG3	1.99	0.44
1:A:1433:MET:HE2	2:B:1145:SER:OG	2.18	0.44
4:D:188:ALA:HB2	4:D:208:GLU:HG3	1.98	0.44
1:A:856:THR:HB	1:A:865:GLN:HB2	2.00	0.43
2:B:211:VAL:HG23	2:B:483:LEU:HB2	2.00	0.43
2:B:848:ARG:HD2	10:J:8:PHE:O	2.17	0.43
1:A:434:ARG:NH2	1:A:440:ASP:OD2	2.51	0.43
1:A:1288:ASP:HA	1:A:1302:PRO:HB3	1.99	0.43
3:C:70:ILE:HD11	3:C:144:ILE:HG12	2.00	0.43
3:C:56:THR:HG22	3:C:57:VAL:H	1.83	0.43
1:A:35:ILE:HG22	1:A:84:ILE:HG23	2.01	0.43
1:A:679:ILE:HG13	1:A:732:LEU:HD12	2.00	0.43
1:A:836:TYR:CZ	1:A:840:ARG:HD2	2.53	0.43
1:A:872:GLY:O	1:A:1057:VAL:HG13	2.18	0.43
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.53	0.43
2:B:168:GLY:H	2:B:450:ALA:HB1	1.83	0.43
2:B:806:THR:HG22	2:B:808:ALA:H	1.83	0.43
3:C:149:LYS:C	3:C:151:GLN:H	2.26	0.43
7:G:62:LEU:HD21	7:G:69:GLU:HB2	2.01	0.43
2:B:617:ARG:HG3	2:B:624:LEU:HD12	2.00	0.43
2:B:844:SER:O	2:B:847:ASP:HB2	2.18	0.43
11:K:33:ILE:HD13	11:K:87:LEU:HD22	1.99	0.43
1:A:287:HIS:O	1:A:290:GLU:HG2	2.18	0.43
3:C:41:ILE:HB	3:C:172:PRO:HG3	2.00	0.43
1:A:154:SER:HB3	1:A:162:VAL:HG23	1.99	0.43
2:B:758:PHE:HB3	2:B:761:HIS:CD2	2.53	0.43
1:A:690:VAL:HG11	1:A:794:PRO:HD3	2.01	0.43
2:B:100:PRO:HG3	2:B:172:ILE:HD12	2.01	0.43
1:A:1193:LEU:HB2	1:A:1260:LEU:HD21	1.99	0.43
11:K:5:ASP:HB3	11:K:7:PHE:CE2	2.54	0.43
1:A:380:VAL:CG1	1:A:385:ILE:HG12	2.49	0.43
2:B:1106:ARG:HG2	2:B:1127:GLY:HA2	2.01	0.43
3:C:66:ARG:HH21	10:J:2:ILE:HG23	1.84	0.43
5:E:56:LYS:HE3	5:E:84:ASP:HB2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:24:LEU:O	10:J:30:LEU:HB2	2.19	0.43
1:A:88:LYS:HB2	1:A:276:LEU:HD21	2.01	0.42
1:A:465:TYR:CE1	11:K:4:PRO:HD2	2.54	0.42
1:A:1442:ASP:HB2	6:F:137:TYR:CE2	2.54	0.42
2:B:101:MET:HG2	2:B:111:ALA:HA	2.01	0.42
2:B:339:THR:CG2	2:B:351:TYR:HE2	2.28	0.42
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	2.01	0.42
1:A:1346:ALA:HB1	5:E:149:LEU:HD22	2.01	0.42
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.54	0.42
1:A:472:LEU:O	1:A:475:THR:HB	2.19	0.42
12:L:60:ARG:NH2	12:L:65:VAL:HG22	2.34	0.42
1:A:590:ARG:NH1	1:A:620:LYS:HD2	2.34	0.42
2:B:315:LYS:HG2	9:I:13:MET:HE1	2.00	0.42
2:B:637:LEU:HD12	2:B:693:ILE:HD13	2.02	0.42
2:B:658:ILE:HG23	2:B:662:MET:HE2	2.02	0.42
3:C:73:GLN:O	3:C:129:ILE:HA	2.20	0.42
1:A:1341:ILE:HG13	1:A:1379:GLY:O	2.20	0.42
7:G:13:LEU:HD23	7:G:13:LEU:HA	1.90	0.42
10:J:48:ARG:HE	10:J:49:MET:HE2	1.85	0.42
15:T:9:DA:H2'	15:T:10:DA:C8	2.55	0.42
1:A:282:ASN:HB3	1:A:283:GLY:H	1.72	0.42
2:B:69:LEU:HD11	2:B:425:THR:HG23	2.01	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.01	0.42
2:B:640:VAL:HG22	2:B:651:LEU:HG	2.00	0.42
6:F:109:VAL:HG11	6:F:123:LYS:HG2	2.01	0.42
1:A:1354:ASN:O	1:A:1358:SER:HB3	2.20	0.42
5:E:156:LEU:HD11	5:E:197:LYS:HB2	2.01	0.42
7:G:119:LEU:HD21	7:G:137:ILE:HD12	2.00	0.42
1:A:1130:GLN:HA	1:A:1133:LEU:HD12	2.01	0.42
2:B:997:GLU:HG2	3:C:39:ALA:HB2	2.01	0.42
4:D:175:PHE:HZ	7:G:85:GLU:HG3	1.84	0.42
1:A:35:ILE:HG21	1:A:241:VAL:HG21	2.01	0.42
1:A:89:PRO:HG2	1:A:204:THR:HB	2.02	0.42
1:A:117:GLU:CD	1:A:117:GLU:H	2.28	0.42
1:A:1436:ILE:O	1:A:1437:GLY:C	2.62	0.42
2:B:101:MET:HB3	2:B:109:THR:HG22	2.01	0.42
2:B:915:THR:HG21	2:B:934:LYS:HB2	2.01	0.42
2:B:1138:MET:HB3	2:B:1147:LEU:HG	2.02	0.42
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.55	0.42
1:A:879:GLU:OE2	1:A:962:ARG:NH2	2.53	0.42
7:G:112:LYS:HA	7:G:115:MET:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:ASP:C	1:A:911:SER:H	2.27	0.41
2:B:21:GLU:O	2:B:656:GLY:HA3	2.20	0.41
2:B:67:SER:HB2	2:B:92:PHE:HD1	1.84	0.41
2:B:287:ARG:HG3	2:B:292:ILE:HA	2.02	0.41
3:C:18:VAL:HG12	3:C:20:PHE:HD1	1.85	0.41
7:G:111:THR:HG22	7:G:113:HIS:N	2.28	0.41
10:J:48:ARG:NH2	10:J:49:MET:HE1	2.35	0.41
15:T:12:DT:H2'	15:T:13:DA:C8	2.55	0.41
1:A:1267:MET:HA	1:A:1271:ILE:HD12	2.01	0.41
2:B:882:THR:C	2:B:884:ARG:H	2.28	0.41
13:N:4:DG:H1	15:T:14:DC:N4	2.14	0.41
1:A:500:GLU:OE1	1:A:1438:THR:HG21	2.20	0.41
1:A:1279:ILE:CD1	1:A:1312:ASN:HB3	2.50	0.41
2:B:343:ILE:O	2:B:344:LYS:HB2	2.20	0.41
3:C:10:ILE:CD1	11:K:108:GLU:HB3	2.50	0.41
4:D:31:GLN:O	4:D:34:GLN:HB2	2.20	0.41
5:E:100:ILE:HA	5:E:105:PHE:HD2	1.85	0.41
8:H:80:ARG:HA	8:H:81:PRO:HD3	1.93	0.41
9:I:85:PHE:HD2	9:I:99:LEU:HD22	1.85	0.41
1:A:78:PRO:HA	2:B:1201:LYS:HZ1	1.85	0.41
1:A:855:THR:HG23	1:A:857:ARG:HG2	2.02	0.41
1:A:1161:THR:HG22	1:A:1163:ILE:O	2.20	0.41
1:A:1430:LEU:O	2:B:1196:ILE:HG22	2.20	0.41
3:C:259:LEU:HD21	11:K:91:CYS:HB3	2.03	0.41
9:I:76:PRO:HD2	9:I:108:HIS:HD2	1.86	0.41
1:A:208:LEU:HG	1:A:235:ILE:HG21	2.01	0.41
3:C:114:TYR:CD1	3:C:140:ASN:HB3	2.56	0.41
10:J:37:SER:OG	10:J:47:ARG:NH2	2.53	0.41
1:A:11:LEU:HD12	2:B:1193:GLN:HG3	2.02	0.41
2:B:492:LEU:HD23	2:B:492:LEU:HA	1.96	0.41
3:C:148:ARG:HG3	3:C:149:LYS:H	1.85	0.41
5:E:215:MET:HE2	5:E:215:MET:HA	2.03	0.41
1:A:49:LYS:HE2	1:A:61:ILE:HB	2.02	0.41
1:A:55:ASP:O	1:A:55:ASP:OD2	2.39	0.41
1:A:185:TRP:H	1:A:185:TRP:HE3	1.68	0.41
1:A:447:GLN:HA	1:A:448:PRO:C	2.46	0.41
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.56	0.41
2:B:834:ASN:HB3	2:B:840:ILE:HG13	2.03	0.41
2:B:941:LEU:HD21	2:B:946:ASN:HA	2.03	0.41
2:B:1106:ARG:NH1	2:B:1125:ASP:O	2.54	0.41
2:B:1181:GLU:N	2:B:1188:LYS:HE3	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:LEU:HD11	5:E:109:ILE:HG13	2.03	0.41
6:F:89:GLU:O	6:F:93:ILE:HD12	2.20	0.41
11:K:51:LEU:CD1	11:K:59:ALA:HB3	2.51	0.41
1:A:1058:VAL:HG12	1:A:1062:GLU:HG3	2.01	0.41
2:B:416:LEU:HD11	2:B:460:ALA:HB3	2.03	0.41
1:A:84:ILE:HG21	1:A:270:LEU:HD21	2.03	0.41
1:A:339:ASN:CB	2:B:1117:GLN:HE22	2.22	0.41
1:A:1218:GLN:HE21	1:A:1218:GLN:HB3	1.70	0.41
2:B:247:GLY:C	2:B:249:ARG:H	2.28	0.41
2:B:309:GLN:HG2	2:B:390:LEU:HD22	2.03	0.41
2:B:763:GLN:HG2	2:B:765:PRO:HD2	2.03	0.41
5:E:46:TYR:HD1	5:E:57:MET:HB3	1.86	0.41
5:E:69:ILE:H	5:E:69:ILE:HG13	1.67	0.41
7:G:150:CYS:HB3	7:G:159:ALA:HB2	2.03	0.41
12:L:38:LEU:HD22	12:L:56:LEU:HD21	2.01	0.41
1:A:1279:ILE:HD11	1:A:1312:ASN:HB3	2.02	0.41
2:B:662:MET:HA	2:B:665:GLU:HB2	2.03	0.41
2:B:792:MET:H	2:B:857:ARG:HA	1.86	0.41
2:B:860:MET:HE3	2:B:860:MET:HB3	2.00	0.41
1:A:1092:LYS:HG3	1:A:1094:VAL:HG23	2.03	0.40
2:B:1207:LEU:HB3	2:B:1212:ILE:HG22	2.02	0.40
5:E:202:SER:HB3	5:E:205:SER:H	1.86	0.40
1:A:1441:PHE:CZ	6:F:89:GLU:HA	2.57	0.40
2:B:1168:LEU:HB2	2:B:1170:THR:OG1	2.22	0.40
3:C:97:VAL:HG11	3:C:130:GLY:HA3	2.03	0.40
10:J:6:ARG:HA	10:J:12:LYS:O	2.21	0.40
10:J:32:GLU:H	10:J:32:GLU:CD	2.30	0.40
13:N:8:DT:O2	15:T:11:DG:N2	2.54	0.40
1:A:54:ASN:HB3	1:A:247:ARG:HH22	1.87	0.40
1:A:372:LYS:HA	1:A:435:HIS:CD2	2.55	0.40
1:A:568:PRO:HG2	8:H:46:LEU:HB3	2.03	0.40
1:A:836:TYR:O	1:A:840:ARG:HD3	2.21	0.40
1:A:1329:THR:H	1:A:1335:ILE:HD11	1.85	0.40
4:D:5:THR:HG21	7:G:74:TYR:OH	2.20	0.40
5:E:102:GLU:C	5:E:104:ASN:H	2.29	0.40
6:F:152:ILE:H	6:F:152:ILE:HG13	1.78	0.40
2:B:658:ILE:HD12	2:B:658:ILE:HA	1.95	0.40
7:G:111:THR:HB	7:G:114:LEU:HD23	2.03	0.40
1:A:75:ASN:O	1:A:76:GLU:HB2	2.22	0.40
1:A:436:ILE:HD12	1:A:436:ILE:HA	1.91	0.40
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:974:ASP:C	1:A:976:THR:H	2.30	0.40
1:A:982:THR:H	1:A:985:ASP:HB2	1.86	0.40
1:A:1312:ASN:ND2	1:A:1315:GLU:HB2	2.36	0.40
7:G:151:ILE:HD11	7:G:160:ILE:HD11	2.03	0.40
10:J:48:ARG:HH21	10:J:49:MET:HE1	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1415/1732 (82%)	1247 (88%)	113 (8%)	55 (4%)	2	15
2	B	1095/1224 (90%)	963 (88%)	94 (9%)	38 (4%)	3	16
3	C	264/318 (83%)	243 (92%)	19 (7%)	2 (1%)	16	44
4	D	174/221 (79%)	154 (88%)	13 (8%)	7 (4%)	2	15
5	E	212/215 (99%)	198 (93%)	12 (6%)	2 (1%)	14	42
6	F	82/155 (53%)	75 (92%)	5 (6%)	2 (2%)	4	22
7	G	169/171 (99%)	156 (92%)	10 (6%)	3 (2%)	6	26
8	H	129/146 (88%)	103 (80%)	17 (13%)	9 (7%)	1	6
9	I	117/122 (96%)	94 (80%)	15 (13%)	8 (7%)	1	6
10	J	63/70 (90%)	52 (82%)	7 (11%)	4 (6%)	1	7
11	K	113/120 (94%)	109 (96%)	4 (4%)	0	100	100
12	L	44/70 (63%)	28 (64%)	8 (18%)	8 (18%)	0	0
All	All	3877/4564 (85%)	3422 (88%)	317 (8%)	138 (4%)	2	16

All (138) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	57	ARG
1	A	74	MET
1	A	76	GLU
1	A	189	ARG
1	A	257	ARG
1	A	286	HIS
1	A	311	GLN
1	A	318	SER
1	A	332	LYS
1	A	335	ARG
1	A	448	PRO
1	A	449	SER
1	A	1281	ARG
1	A	1403	GLU
1	A	1405	THR
2	B	229	ALA
2	B	307	ASP
2	B	341	LEU
2	B	344	LYS
2	B	476	ARG
2	B	707	PRO
2	B	731	VAL
2	B	867	GLY
2	B	1066	SER
2	B	1176	ASN
4	D	18	VAL
4	D	199	ASN
10	J	55	ASP
12	L	50	ASP
12	L	53	HIS
12	L	56	LEU
1	A	35	ILE
1	A	54	ASN
1	A	58	LEU
1	A	69	THR
1	A	166	GLY
1	A	169	ASN
1	A	178	GLY
1	A	193	ASP
1	A	195	ASP
1	A	331	GLY
1	A	628	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	775	ILE
1	A	1175	SER
1	A	1377	THR
2	B	108	VAL
2	B	340	ALA
2	B	368	GLU
2	B	575	PRO
2	B	629	ASP
2	B	751	VAL
2	B	792	MET
2	B	879	ARG
2	B	1157	ALA
2	B	1175	LEU
2	B	1181	GLU
4	D	119	ARG
4	D	220	LEU
5	E	45	LYS
6	F	78	GLN
9	I	9	ASP
9	I	95	THR
10	J	6	ARG
1	A	43	GLU
1	A	47	ARG
1	A	569	LYS
1	A	1124	HIS
1	A	1173	HIS
1	A	1221	LYS
2	B	282	ILE
2	B	447	ALA
2	B	711	GLU
2	B	881	ASN
2	B	883	LEU
2	B	960	GLY
2	B	1155	SER
6	F	73	ALA
8	H	60	ALA
8	H	82	PRO
8	H	90	ALA
9	I	60	GLN
9	I	113	ASP
10	J	2	ILE
12	L	28	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	45	ALA
1	A	70	CYS
1	A	155	GLU
1	A	167	CYS
1	A	192	GLY
1	A	336	ILE
1	A	399	HIS
1	A	567	LYS
1	A	958	VAL
1	A	1365	TYR
2	B	1046	PRO
4	D	13	ARG
4	D	169	SER
5	E	36	GLU
7	G	63	PRO
7	G	154	VAL
8	H	81	PRO
8	H	83	GLN
8	H	128	ASN
9	I	105	SER
12	L	26	THR
12	L	54	ARG
12	L	59	ALA
1	A	65	LEU
1	A	333	GLU
1	A	1255	GLU
2	B	67	SER
7	G	139	ILE
8	H	17	PRO
8	H	18	GLY
9	I	3	THR
9	I	115	LYS
10	J	17	LYS
1	A	41	MET
1	A	55	ASP
1	A	310	GLY
2	B	249	ARG
2	B	959	ASP
2	B	1017	ILE
2	B	1108	ARG
4	D	16	LYS
8	H	77	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	385	ILE
1	A	312	PRO
2	B	364	ILE
1	A	1437	GLY
2	B	436	VAL
2	B	992	ILE
2	B	247	GLY
3	C	150	GLY
9	I	58	VAL
1	A	910	PRO
3	C	240	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1241/1519 (82%)	1040 (84%)	201 (16%)	2	10
2	B	966/1061 (91%)	838 (87%)	128 (13%)	4	15
3	C	234/274 (85%)	203 (87%)	31 (13%)	4	16
4	D	160/200 (80%)	124 (78%)	36 (22%)	1	3
5	E	196/197 (100%)	169 (86%)	27 (14%)	3	14
6	F	74/137 (54%)	65 (88%)	9 (12%)	5	19
7	G	152/152 (100%)	128 (84%)	24 (16%)	2	10
8	H	117/128 (91%)	102 (87%)	15 (13%)	4	17
9	I	113/116 (97%)	100 (88%)	13 (12%)	5	20
10	J	60/65 (92%)	44 (73%)	16 (27%)	0	1
11	K	99/102 (97%)	83 (84%)	16 (16%)	2	10
12	L	40/57 (70%)	29 (72%)	11 (28%)	0	1
All	All	3452/4008 (86%)	2925 (85%)	527 (15%)	3	10

All (527) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	15	LYS
1	A	34	LYS
1	A	41	MET
1	A	45	GLN
1	A	53	LEU
1	A	62	ASP
1	A	64	ASN
1	A	65	LEU
1	A	70	CYS
1	A	90	VAL
1	A	93	VAL
1	A	96	ILE
1	A	126	LEU
1	A	132	LYS
1	A	147	VAL
1	A	152	VAL
1	A	163	SER
1	A	174	ILE
1	A	182	VAL
1	A	188	ASP
1	A	195	ASP
1	A	199	LEU
1	A	204	THR
1	A	208	LEU
1	A	220	THR
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	252	PHE
1	A	253	ASN
1	A	256	GLN
1	A	261	ASP
1	A	270	LEU
1	A	279	LEU
1	A	291	GLU
1	A	295	LEU
1	A	307	ASP
1	A	311	GLN
1	A	315	LEU
1	A	322	VAL
1	A	324	SER
1	A	330	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	335	ARG
1	A	337	ARG
1	A	344	ARG
1	A	353	ILE
1	A	375	THR
1	A	379	VAL
1	A	381	THR
1	A	385	ILE
1	A	386	ASP
1	A	393	ARG
1	A	397	ASN
1	A	398	GLU
1	A	407	ARG
1	A	408	ASP
1	A	423	ASP
1	A	424	ILE
1	A	425	GLN
1	A	427	GLN
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	445	ASN
1	A	448	PRO
1	A	450	LEU
1	A	451	HIS
1	A	454	SER
1	A	461	LYS
1	A	463	ILE
1	A	469	ARG
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	489	LEU
1	A	496	GLU
1	A	500	GLU
1	A	505	CYS
1	A	513	SER
1	A	517	ASN
1	A	518	LYS
1	A	532	ARG
1	A	538	ASP
1	A	544	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	566	ILE
1	A	571	LEU
1	A	577	ILE
1	A	589	GLN
1	A	593	GLU
1	A	597	LEU
1	A	598	LEU
1	A	603	ASN
1	A	613	ILE
1	A	618	GLU
1	A	622	VAL
1	A	629	LEU
1	A	634	THR
1	A	635	ARG
1	A	640	GLN
1	A	664	THR
1	A	666	ILE
1	A	672	ASP
1	A	685	GLU
1	A	702	LEU
1	A	719	VAL
1	A	738	LYS
1	A	756	ILE
1	A	764	CYS
1	A	768	GLN
1	A	769	SER
1	A	773	LYS
1	A	782	ARG
1	A	788	SER
1	A	795	GLU
1	A	811	GLN
1	A	821	ARG
1	A	826	ASP
1	A	831	THR
1	A	839	ARG
1	A	846	GLU
1	A	849	MET
1	A	855	THR
1	A	856	THR
1	A	867	ILE
1	A	878	ILE
1	A	885	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	886	ILE
1	A	889	SER
1	A	904	THR
1	A	919	ILE
1	A	920	LEU
1	A	926	GLN
1	A	929	LEU
1	A	948	VAL
1	A	960	ILE
1	A	964	ILE
1	A	973	ILE
1	A	983	ILE
1	A	988	LEU
1	A	991	LYS
1	A	998	LEU
1	A	1001	ARG
1	A	1015	VAL
1	A	1040	GLN
1	A	1052	GLN
1	A	1058	VAL
1	A	1080	THR
1	A	1116	LEU
1	A	1118	VAL
1	A	1121	GLU
1	A	1124	HIS
1	A	1135	ARG
1	A	1146	VAL
1	A	1168	GLU
1	A	1169	ILE
1	A	1170	ILE
1	A	1173	HIS
1	A	1176	LEU
1	A	1193	LEU
1	A	1195	LEU
1	A	1208	THR
1	A	1218	GLN
1	A	1223	ASP
1	A	1237	ILE
1	A	1242	VAL
1	A	1255	GLU
1	A	1257	ASP
1	A	1260	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1264	GLU
1	A	1276	VAL
1	A	1279	ILE
1	A	1281	ARG
1	A	1289	ARG
1	A	1291	VAL
1	A	1295	THR
1	A	1301	GLU
1	A	1308	THR
1	A	1309	ASP
1	A	1314	SER
1	A	1325	THR
1	A	1327	ILE
1	A	1333	ILE
1	A	1335	ILE
1	A	1341	ILE
1	A	1356	ILE
1	A	1370	LEU
1	A	1376	THR
1	A	1387	HIS
1	A	1391	ARG
1	A	1405	THR
1	A	1411	GLU
1	A	1420	ASP
1	A	1425	SER
1	A	1426	GLU
1	A	1433	MET
1	A	1442	ASP
1	A	1444	MET
1	A	1445	ILE
1	A	1451	VAL
1	A	1454	MET
2	B	25	ILE
2	B	46	GLN
2	B	63	ILE
2	B	109	THR
2	B	110	HIS
2	B	118	ARG
2	B	119	LEU
2	B	128	LEU
2	B	134	LYS
2	B	178	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	187	SER
2	B	225	VAL
2	B	234	ILE
2	B	251	ILE
2	B	261	ARG
2	B	272	THR
2	B	278	GLN
2	B	287	ARG
2	B	294	ASP
2	B	313	MET
2	B	324	ILE
2	B	336	ARG
2	B	337	ARG
2	B	339	THR
2	B	341	LEU
2	B	343	ILE
2	B	344	LYS
2	B	346	GLU
2	B	347	LYS
2	B	348	ARG
2	B	357	GLN
2	B	361	LEU
2	B	365	THR
2	B	387	LEU
2	B	393	LYS
2	B	398	ARG
2	B	408	LEU
2	B	412	LEU
2	B	416	LEU
2	B	423	LYS
2	B	429	PHE
2	B	446	LEU
2	B	448	ILE
2	B	453	ILE
2	B	461	LEU
2	B	470	LYS
2	B	485	ARG
2	B	537	LYS
2	B	543	SER
2	B	545	ILE
2	B	547	VAL
2	B	552	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	570	VAL
2	B	574	SER
2	B	602	THR
2	B	604	ARG
2	B	609	ILE
2	B	614	SER
2	B	615	MET
2	B	616	ILE
2	B	620	ARG
2	B	628	THR
2	B	642	ASP
2	B	644	GLU
2	B	651	LEU
2	B	653	VAL
2	B	658	ILE
2	B	668	ASP
2	B	678	GLU
2	B	690	VAL
2	B	708	GLU
2	B	709	ASP
2	B	723	VAL
2	B	729	ILE
2	B	731	VAL
2	B	736	THR
2	B	766	ARG
2	B	786	ASN
2	B	787	VAL
2	B	790	ASP
2	B	795	ILE
2	B	835	GLN
2	B	839	MET
2	B	853	SER
2	B	871	THR
2	B	873	THR
2	B	878	GLN
2	B	881	ASN
2	B	882	THR
2	B	889	THR
2	B	918	ILE
2	B	933	SER
2	B	953	LEU
2	B	964	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	972	LYS
2	B	975	GLN
2	B	983	ARG
2	B	986	GLN
2	B	997	GLU
2	B	1007	VAL
2	B	1010	LEU
2	B	1017	ILE
2	B	1020	ARG
2	B	1028	GLU
2	B	1045	SER
2	B	1050	ILE
2	B	1060	ARG
2	B	1065	GLN
2	B	1072	MET
2	B	1079	LYS
2	B	1094	ARG
2	B	1106	ARG
2	B	1113	VAL
2	B	1123	SER
2	B	1133	MET
2	B	1138	MET
2	B	1147	LEU
2	B	1151	LEU
2	B	1160	VAL
2	B	1169	MET
2	B	1175	LEU
2	B	1183	LYS
2	B	1188	LYS
2	B	1189	ILE
2	B	1191	ILE
2	B	1201	LYS
2	B	1202	LEU
2	B	1212	ILE
3	C	11	ARG
3	C	12	GLU
3	C	16	ASP
3	C	22	LEU
3	C	23	SER
3	C	25	VAL
3	C	26	ASP
3	C	52	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	53	THR
3	C	55	THR
3	C	56	THR
3	C	70	ILE
3	C	84	ARG
3	C	100	THR
3	C	101	LEU
3	C	106	GLU
3	C	108	GLU
3	C	119	VAL
3	C	125	MET
3	C	127	ARG
3	C	129	ILE
3	C	133	ILE
3	C	155	LEU
3	C	166	GLU
3	C	224	GLN
3	C	226	ASP
3	C	235	VAL
3	C	238	ILE
3	C	240	VAL
3	C	259	LEU
3	C	268	ASP
4	D	5	THR
4	D	7	THR
4	D	9	GLN
4	D	10	THR
4	D	12	ARG
4	D	18	VAL
4	D	22	GLU
4	D	23	ASN
4	D	27	LEU
4	D	28	GLN
4	D	32	GLU
4	D	40	HIS
4	D	41	GLN
4	D	47	LEU
4	D	50	LEU
4	D	53	SER
4	D	67	ARG
4	D	118	THR
4	D	119	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	126	ILE
4	D	127	ASP
4	D	134	THR
4	D	137	ASN
4	D	139	LYS
4	D	153	ARG
4	D	155	ARG
4	D	156	ASP
4	D	158	GLU
4	D	177	VAL
4	D	187	THR
4	D	197	SER
4	D	205	ASP
4	D	206	GLU
4	D	213	GLU
4	D	217	LEU
4	D	221	TYR
5	E	8	ASN
5	E	30	ILE
5	E	31	THR
5	E	37	LEU
5	E	45	LYS
5	E	57	MET
5	E	67	GLU
5	E	69	ILE
5	E	81	GLU
5	E	92	THR
5	E	98	ILE
5	E	99	HIS
5	E	104	ASN
5	E	114	ASN
5	E	131	THR
5	E	157	SER
5	E	166	LYS
5	E	173	SER
5	E	177	ARG
5	E	184	VAL
5	E	190	LEU
5	E	191	LYS
5	E	192	ARG
5	E	196	VAL
5	E	202	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	204	THR
5	E	210	SER
6	F	82	THR
6	F	93	ILE
6	F	103	MET
6	F	109	VAL
6	F	115	THR
6	F	122	MET
6	F	123	LYS
6	F	127	GLU
6	F	152	ILE
7	G	13	LEU
7	G	22	MET
7	G	24	GLN
7	G	26	LEU
7	G	29	LYS
7	G	33	GLU
7	G	34	VAL
7	G	35	GLU
7	G	61	ILE
7	G	83	LYS
7	G	85	GLU
7	G	90	THR
7	G	92	VAL
7	G	93	SER
7	G	96	GLN
7	G	119	LEU
7	G	134	GLU
7	G	138	THR
7	G	143	ILE
7	G	150	CYS
7	G	151	ILE
7	G	154	VAL
7	G	158	HIS
7	G	163	ILE
8	H	12	VAL
8	H	13	SER
8	H	14	GLU
8	H	26	ILE
8	H	39	THR
8	H	42	ILE
8	H	89	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	91	ASP
8	H	94	ASP
8	H	103	LYS
8	H	106	GLU
8	H	128	ASN
8	H	130	ARG
8	H	135	LEU
8	H	138	GLU
9	I	7	CYS
9	I	8	ARG
9	I	31	THR
9	I	35	VAL
9	I	43	VAL
9	I	50	THR
9	I	55	THR
9	I	74	GLU
9	I	81	ARG
9	I	83	ASN
9	I	84	VAL
9	I	94	ASP
9	I	120	GLN
10	J	3	VAL
10	J	12	LYS
10	J	13	VAL
10	J	14	VAL
10	J	20	SER
10	J	22	LEU
10	J	23	ASN
10	J	24	LEU
10	J	27	GLU
10	J	29	GLU
10	J	36	LEU
10	J	37	SER
10	J	42	LYS
10	J	48	ARG
10	J	50	ILE
10	J	59	LYS
11	K	1	MET
11	K	11	LEU
11	K	12	LEU
11	K	18	LYS
11	K	20	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	K	25	THR
11	K	29	ASN
11	K	34	THR
11	K	37	LYS
11	K	42	LEU
11	K	47	ARG
11	K	51	LEU
11	K	76	GLN
11	K	79	GLU
11	K	101	LEU
11	K	114	LEU
12	L	27	LEU
12	L	33	GLU
12	L	38	LEU
12	L	40	LEU
12	L	42	ARG
12	L	46	VAL
12	L	54	ARG
12	L	55	ILE
12	L	58	LYS
12	L	61	THR
12	L	68	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	124	GLN
1	A	256	GLN
1	A	282	ASN
1	A	399	HIS
1	A	425	GLN
1	A	451	HIS
1	A	517	ASN
1	A	548	ASN
1	A	700	ASN
1	A	741	ASN
1	A	811	GLN
1	A	935	GLN
1	A	969	GLN
1	A	975	HIS
1	A	994	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1070	GLN
1	A	1106	ASN
1	A	1173	HIS
1	A	1187	GLN
1	A	1203	ASN
1	A	1312	ASN
1	A	1390	ASN
2	B	115	GLN
2	B	206	ASN
2	B	357	GLN
2	B	383	ASN
2	B	433	GLN
2	B	531	GLN
2	B	587	HIS
2	B	592	ASN
2	B	686	ASN
2	B	786	ASN
2	B	843	GLN
2	B	957	ASN
2	B	975	GLN
2	B	1084	GLN
2	B	1117	GLN
2	B	1195	HIS
3	C	7	GLN
3	C	17	ASN
3	C	54	ASN
3	C	73	GLN
3	C	135	GLN
3	C	151	GLN
3	C	224	GLN
3	C	231	ASN
4	D	9	GLN
5	E	5	ASN
5	E	54	GLN
5	E	115	ASN
5	E	146	HIS
7	G	53	ASN
8	H	33	GLN
8	H	131	ASN
8	H	137	GLN
8	H	139	ASN
9	I	60	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	108	HIS
11	K	29	ASN
11	K	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	P	3/5 (60%)	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	$\# Z > 2$
15	BRU	T	22	14,15	18,21,22	0.75	1 (5%)	25,30,33	1.96	6 (24%)

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
15	BRU	T	22	14,15	-	0/7/21/22	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	T	22	BRU	C6-C5	2.06	1.38	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	T	22	BRU	C5-C4-N3	4.58	118.61	113.34
15	T	22	BRU	C4-N3-C2	-4.06	122.02	127.34
15	T	22	BRU	N3-C2-N1	3.87	119.93	114.89
15	T	22	BRU	O4'-C1'-N1	3.75	114.52	107.86
15	T	22	BRU	O4-C4-C5	-3.49	121.35	125.80
15	T	22	BRU	O2-C2-N3	-2.96	116.03	121.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\# Z > 2$
18	APC	P	1011	-	29,33,33	2.37	7 (24%)	44,52,52	2.00	11 (25%)

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
18	APC	P	1011	-	-	0/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	P	1011	APC	PB-O3B	8.96	1.68	1.58
18	P	1011	APC	PA-O1A	4.33	1.61	1.51
18	P	1011	APC	PG-O1G	4.20	1.63	1.50
18	P	1011	APC	C5-C4	2.82	1.44	1.39
18	P	1011	APC	PB-O2B	2.50	1.62	1.56
18	P	1011	APC	PG-O2G	2.42	1.63	1.54
18	P	1011	APC	PA-O2A	-2.31	1.50	1.56

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	P	1011	APC	C5-C4-N3	-6.21	118.17	126.72
18	P	1011	APC	N3-C4-N9	4.61	135.01	127.17
18	P	1011	APC	C4-C5-N7	-4.08	105.92	110.58
18	P	1011	APC	C5-N7-C8	4.05	109.81	103.45
18	P	1011	APC	N3-C2-N1	-3.81	122.81	128.58
18	P	1011	APC	C2-N3-C4	3.74	120.96	111.83
18	P	1011	APC	O2G-PG-O3B	2.93	114.48	104.64
18	P	1011	APC	O4'-C1'-N9	2.27	112.44	108.09
18	P	1011	APC	PB-O3B-PG	-2.25	124.38	132.45
18	P	1011	APC	O2'-C2'-C3'	2.17	118.76	111.82
18	P	1011	APC	N9-C8-N7	-2.03	111.05	113.94

There are no chirality outliers.

There are no torsion outliers.

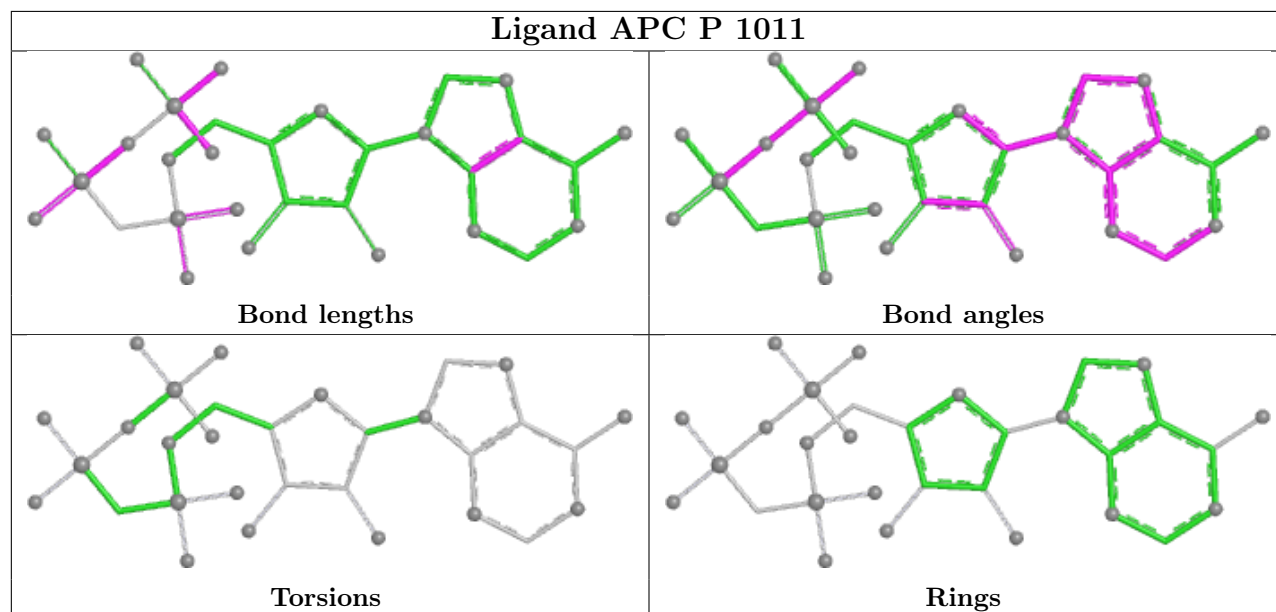
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	P	1011	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	934:LYS	C	935:ARG	N	5.31
1	B	351:TYR	C	352:ALA	N	3.13

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1423/1732 (82%)	-0.22	19 (1%) 75 61	65, 110, 174, 230	0
2	B	1115/1224 (91%)	-0.01	38 (3%) 48 35	66, 124, 185, 221	0
3	C	266/318 (83%)	-0.44	0 100 100	81, 107, 150, 180	0
4	D	178/221 (80%)	-0.04	11 (6%) 26 21	86, 123, 174, 194	0
5	E	214/215 (99%)	-0.08	5 (2%) 61 46	88, 150, 192, 202	0
6	F	84/155 (54%)	-0.57	1 (1%) 76 63	64, 92, 119, 142	0
7	G	171/171 (100%)	-0.24	0 100 100	84, 107, 145, 165	0
8	H	133/146 (91%)	0.39	8 (6%) 27 21	123, 155, 192, 207	0
9	I	119/122 (97%)	0.27	9 (7%) 20 17	114, 156, 190, 213	0
10	J	65/70 (92%)	-0.17	2 (3%) 51 38	88, 108, 145, 161	0
11	K	115/120 (95%)	-0.48	1 (0%) 81 68	80, 110, 147, 166	0
12	L	46/70 (65%)	0.94	5 (10%) 10 11	93, 184, 198, 207	0
13	N	8/14 (57%)	1.85	4 (50%) 0 0	214, 229, 237, 240	0
14	P	4/5 (80%)	0.11	0 100 100	146, 154, 170, 189	0
15	T	17/26 (65%)	1.49	4 (23%) 2 3	156, 210, 225, 227	0
All	All	3958/4609 (85%)	-0.11	107 (2%) 56 42	64, 119, 185, 240	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	27	LEU	6.8
2	B	502	ILE	6.1
2	B	509	ALA	5.6
8	H	63	LEU	5.5
2	B	709	ASP	5.4
2	B	708	GLU	5.3
2	B	446	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1224	PHE	4.9
15	T	25	DT	4.8
2	B	883	LEU	4.6
4	D	24	ALA	4.4
4	D	3	VAL	4.3
2	B	70	ILE	4.3
4	D	20	GLU	4.1
2	B	882	THR	3.9
11	K	114	LEU	3.9
12	L	28	LYS	3.8
2	B	251	ILE	3.7
6	F	72	LYS	3.7
2	B	715	ALA	3.6
1	A	1243	VAL	3.6
2	B	134	LYS	3.6
2	B	343	ILE	3.6
2	B	473	MET	3.4
1	A	51	GLY	3.2
2	B	243	ALA	3.2
12	L	25	ALA	3.1
2	B	918	ILE	3.1
1	A	1081	LEU	3.1
1	A	56	PRO	3.0
2	B	244	LEU	3.0
1	A	1093	LYS	2.9
1	A	251	SER	2.9
2	B	436	VAL	2.9
8	H	90	ALA	2.9
12	L	26	THR	2.9
4	D	221	TYR	2.9
2	B	933	SER	2.8
10	J	65	PRO	2.8
1	A	1187	GLN	2.8
15	T	16	DT	2.7
1	A	194	ALA	2.7
13	N	3	DA	2.7
2	B	20	ASP	2.7
2	B	245	GLU	2.7
9	I	56	ALA	2.7
4	D	18	VAL	2.7
2	B	880	THR	2.6
2	B	341	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	110	PHE	2.6
1	A	310	GLY	2.6
8	H	2	SER	2.6
2	B	351	TYR	2.6
1	A	186	LYS	2.6
1	A	190	ALA	2.6
1	A	1455	PRO	2.6
9	I	120	GLN	2.6
4	D	13	ARG	2.6
5	E	126	SER	2.6
2	B	250	PHE	2.5
2	B	164	LYS	2.5
2	B	447	ALA	2.5
4	D	10	THR	2.5
9	I	50	THR	2.5
2	B	934	LYS	2.5
4	D	76	LYS	2.5
1	A	1095	THR	2.5
12	L	53	HIS	2.5
1	A	257	ARG	2.4
1	A	292	ALA	2.4
8	H	84	ALA	2.4
2	B	723	VAL	2.4
1	A	567	LYS	2.4
2	B	467	GLY	2.4
1	A	640	GLN	2.4
15	T	17	DT	2.4
9	I	93	LYS	2.4
13	N	5	DT	2.4
4	D	187	THR	2.3
4	D	173	HIS	2.3
5	E	114	ASN	2.3
9	I	4	PHE	2.3
2	B	881	ASN	2.3
9	I	2	THR	2.3
10	J	12	LYS	2.3
2	B	1173	ALA	2.2
13	N	6	DA	2.2
15	T	10	DA	2.2
2	B	963	PHE	2.2
2	B	917	PRO	2.2
4	D	118	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
8	H	139	ASN	2.2
13	N	7	DC	2.2
9	I	117	LYS	2.1
9	I	118	ARG	2.1
2	B	340	ALA	2.1
1	A	252	PHE	2.1
2	B	108	VAL	2.1
8	H	46	LEU	2.1
5	E	194	GLU	2.1
9	I	100	PHE	2.1
2	B	1019	SER	2.1
5	E	93	MET	2.1
8	H	138	GLU	2.1
8	H	132	LEU	2.0
1	A	59	GLY	2.0
2	B	272	THR	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
15	BRU	T	22	20/21	0.93	0.09	170,185,187,190	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.

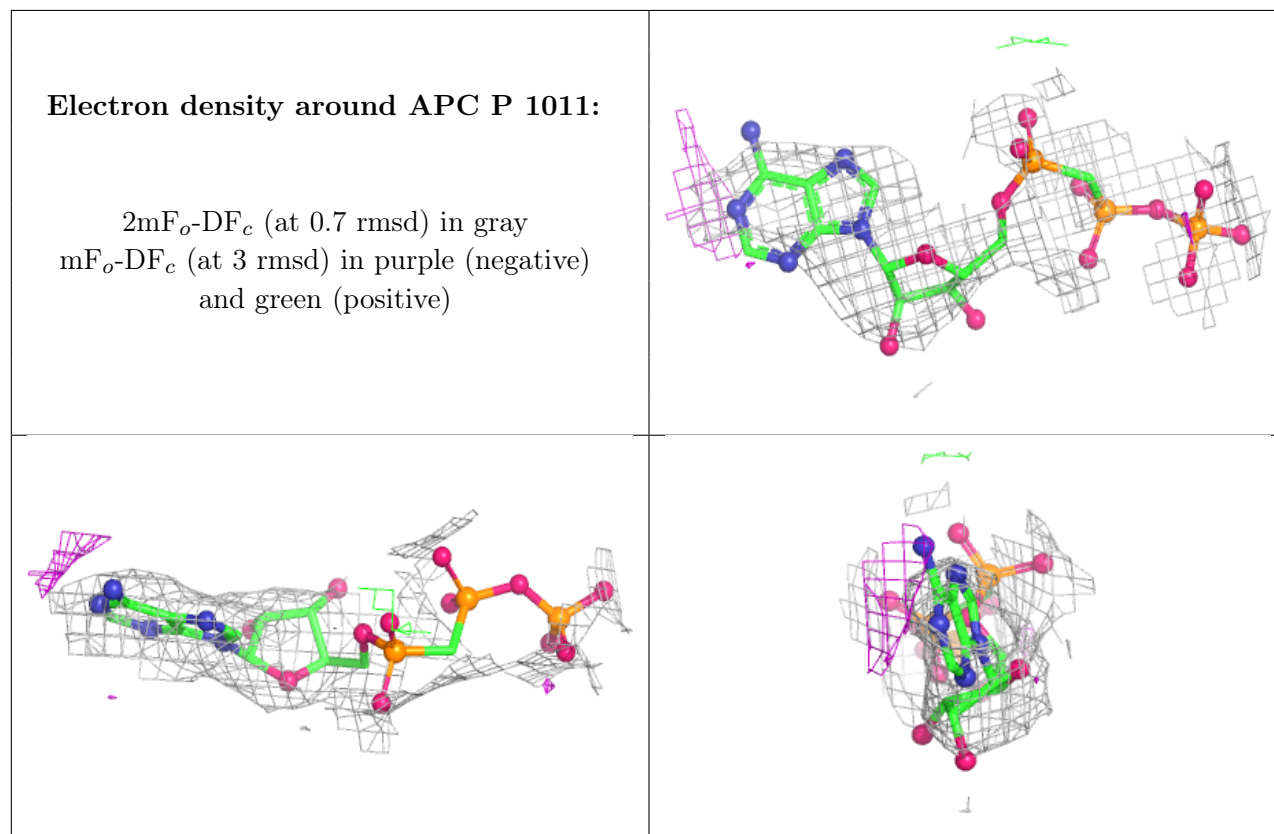
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
18	APC	P	1011	31/31	0.87	0.14	195,198,211,212	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
16	ZN	L	1071	1/1	0.99	0.05	198,198,198,198	0
17	MG	A	2458	1/1	0.99	0.05	110,110,110,110	0
16	ZN	I	1122	1/1	0.99	0.03	191,191,191,191	0
16	ZN	I	1121	1/1	1.00	0.05	130,130,130,130	0
16	ZN	A	2456	1/1	1.00	0.01	138,138,138,138	0
16	ZN	J	1066	1/1	1.00	0.04	98,98,98,98	0
16	ZN	A	2457	1/1	1.00	0.02	85,85,85,85	0
16	ZN	B	2225	1/1	1.00	0.04	95,95,95,95	0
16	ZN	C	1269	1/1	1.00	0.03	96,96,96,96	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 ⓘ

There are no such residues in this entry.