Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 07:26 PM EDT

PDB ID	:	6UPZ
Title	:	RNA polymerase II elongation complex with 5-guanidinohydantoin lesion in state 3
Authors	:	Oh, J.; Wang, D.
Deposited on	:	2019-10-18
Resolution	:	3.10 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:

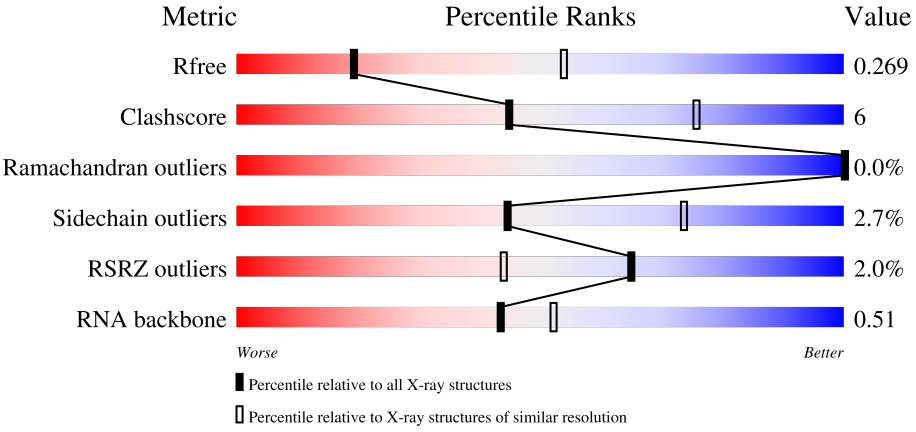
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



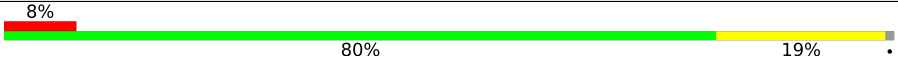
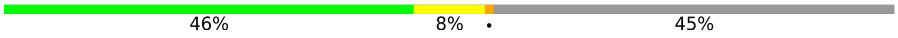
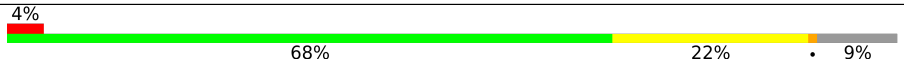
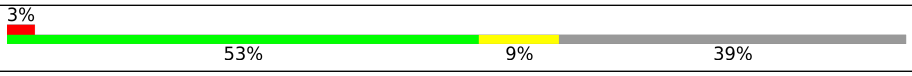
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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 <=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	10	30% 70%
2	T	29	10% 69% 17% 10%
3	N	18	11% 67% 17% 17%
4	A	1733	2% 64% 15% 20%

Continued on next page...

Continued from previous page...

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 (i)

There are 16 unique types of molecules in this entry. The entry contains 29075 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	10	Total	C	N	O	P	0	0	0
			221	98	45	68	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	26	Total	C	N	O	P	0	0	0
			520	249	80	165	26			

- 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	1382	Total	C	N	O	S	0	0	0
			10820	6824	1895	2041	60			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1123	Total	C	N	O	S	0	0	0
			8859	5607	1552	1647	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	212	Total	C	N	O	S	0	0	0
			1731	1100	305	315	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
			1064	670	179	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	118	Total	C	N	O	S	0	0	0
			952	585	173	184	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			

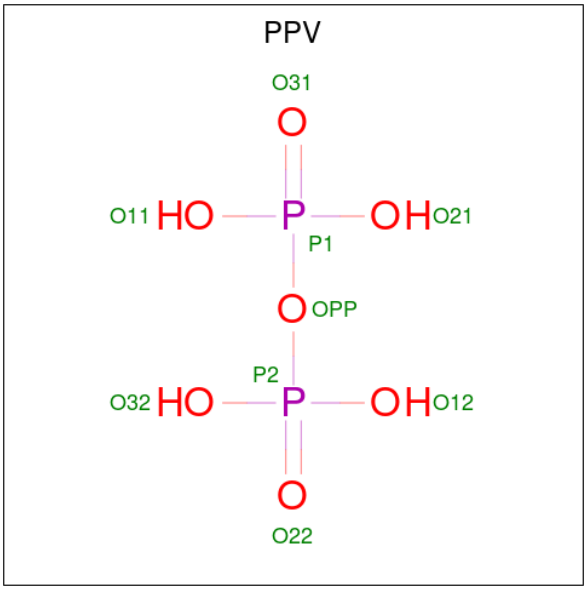
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 16 is PYROPHOSPHATE (three-letter code: PPV) (formula: $H_4O_7P_2$) (labeled as "Ligand of Interest" by depositor).



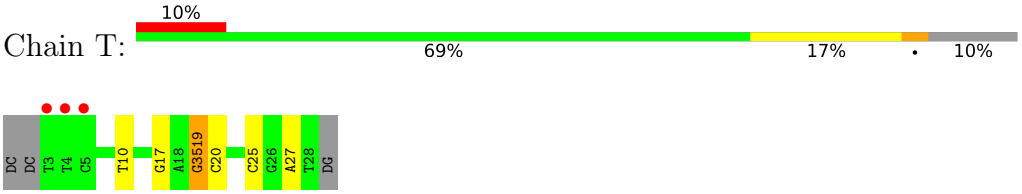
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	B	1	Total O P 9 7 2	0	0

3 Residue-property plots (i)

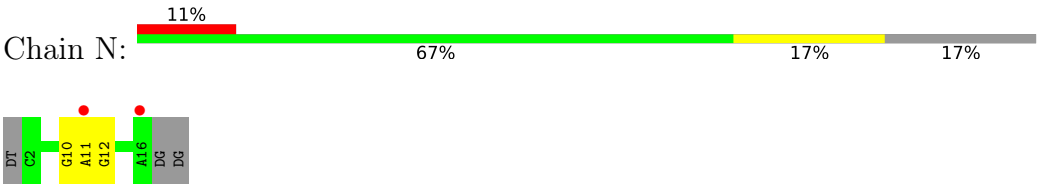
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

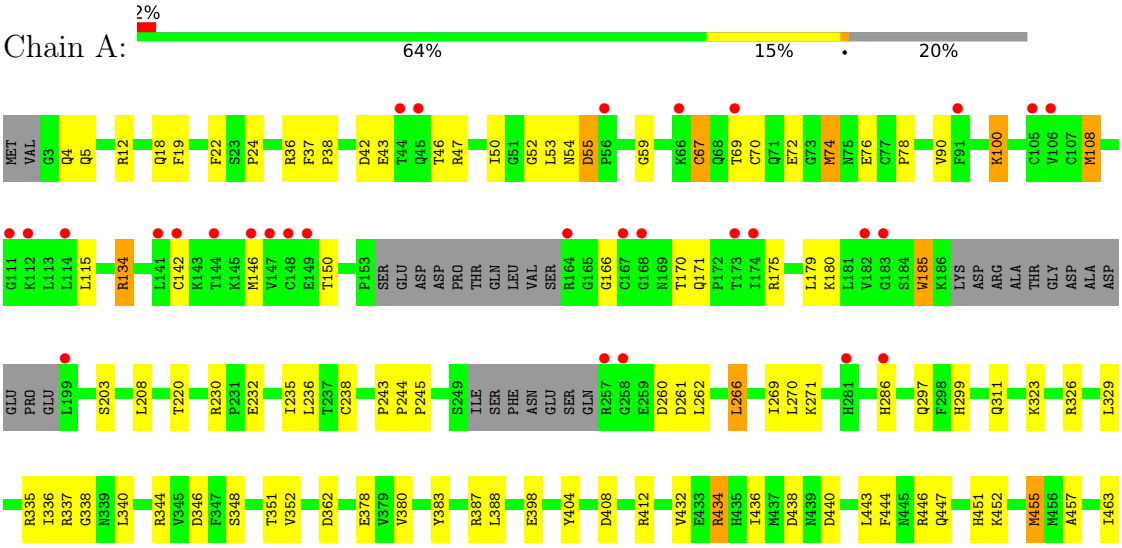
• Molecule 2: Template strand DNA

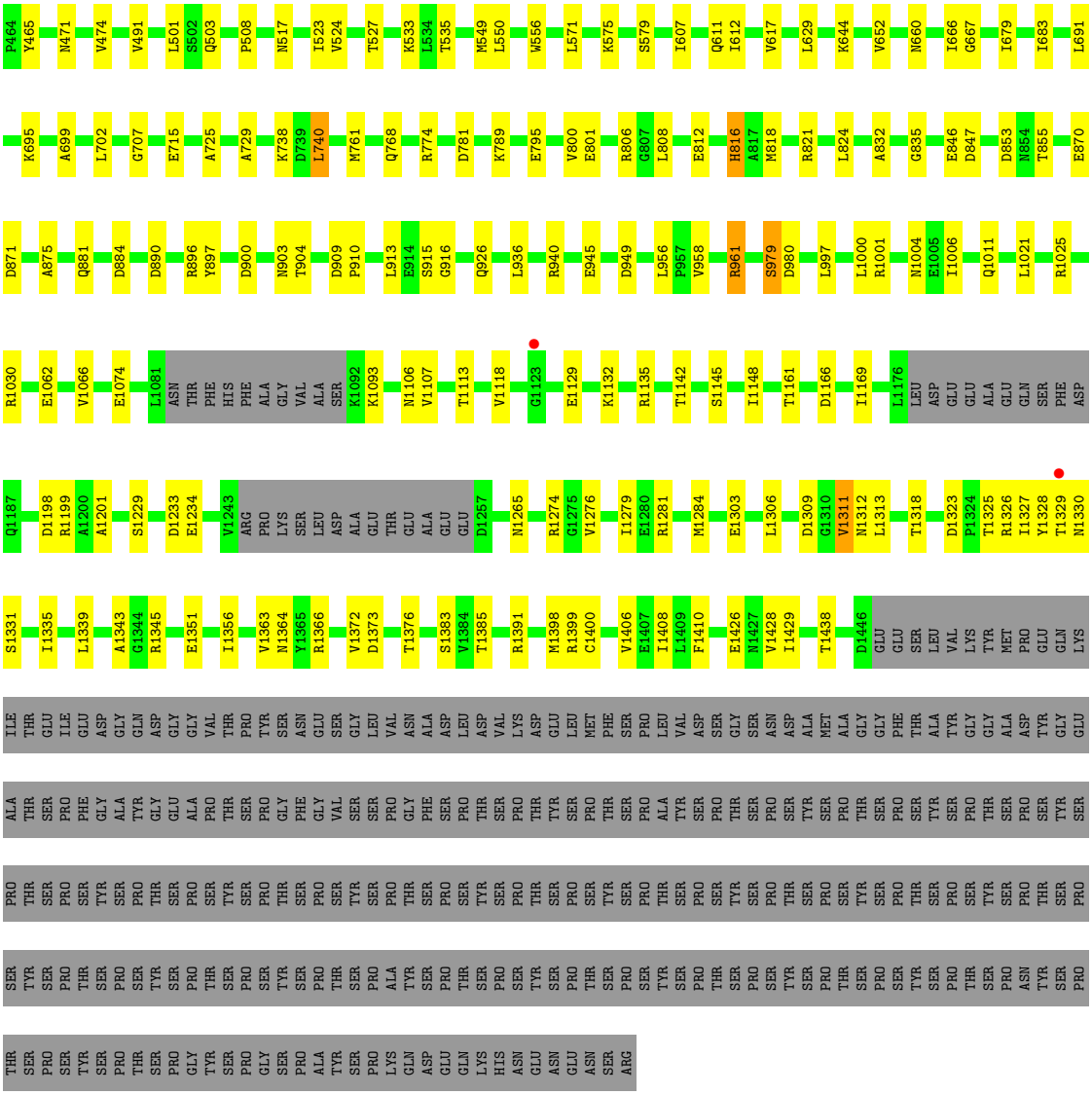


• Molecule 3: Non-template strand DNA



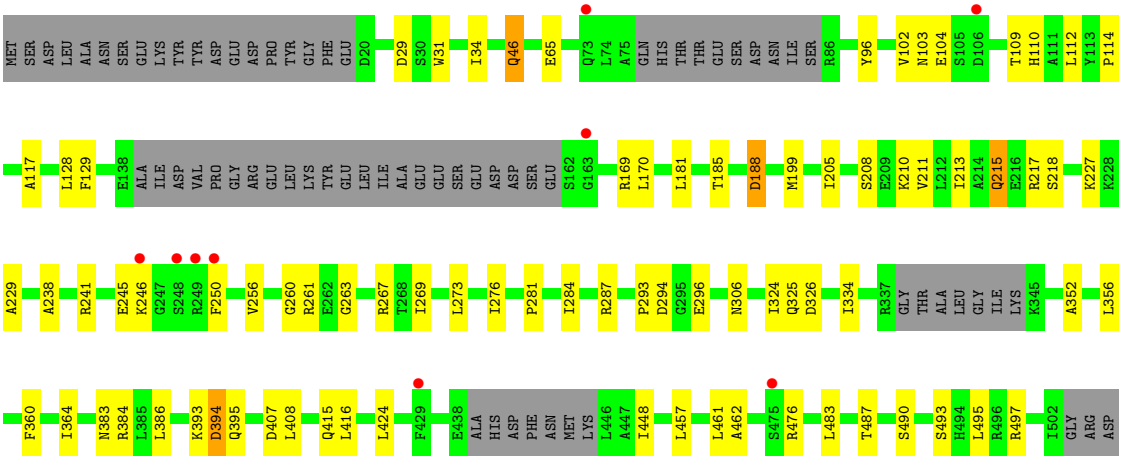
• Molecule 4: DNA-directed RNA polymerase II subunit RPB1

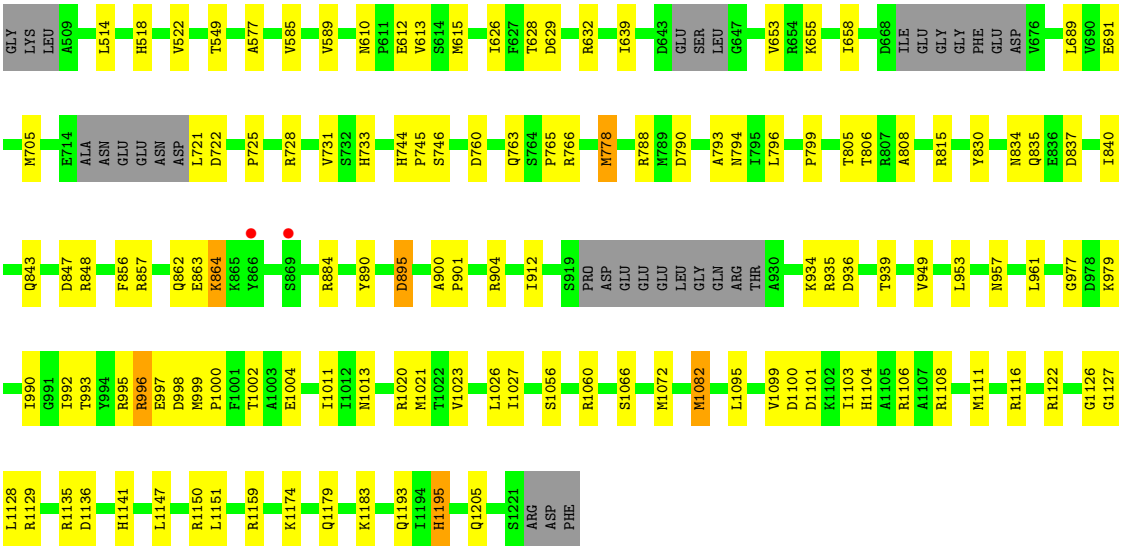




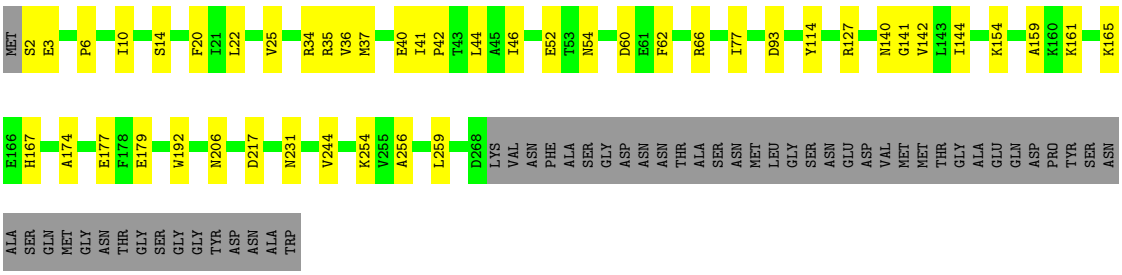
• Molecule 5: DNA-directed RNA polymerase II subunit RPB2

Chain B:

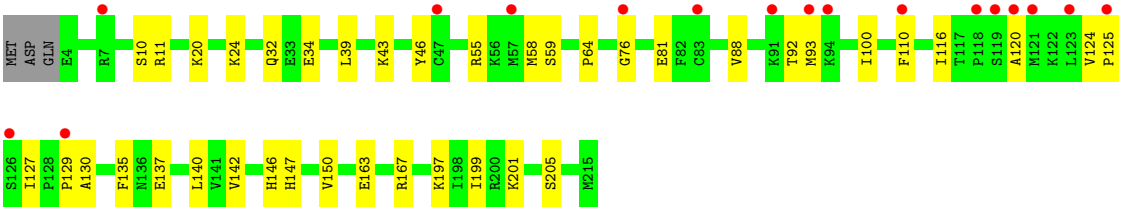




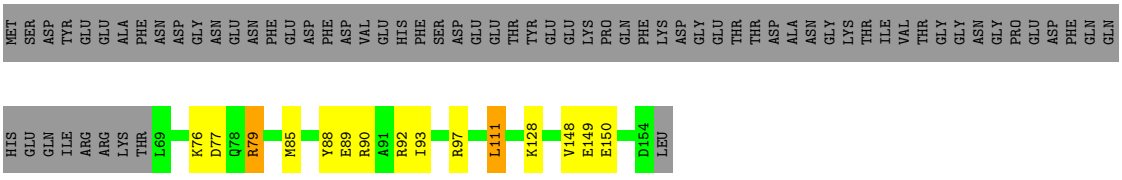
• Molecule 6: DNA-directed RNA polymerase II subunit RPB3



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

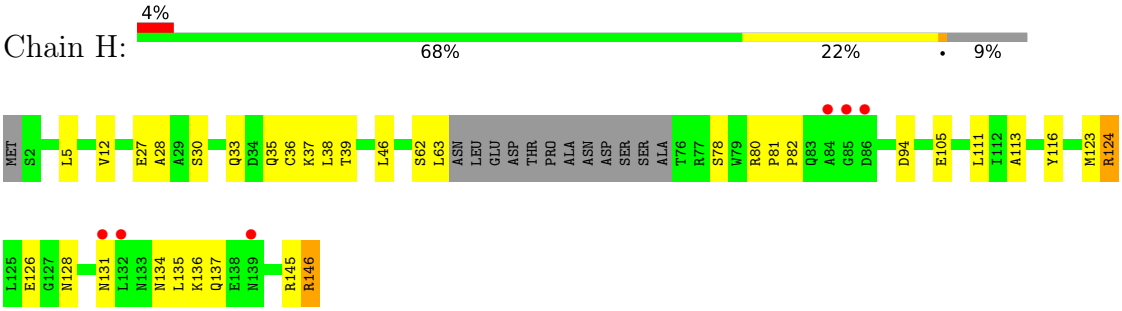


• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC2



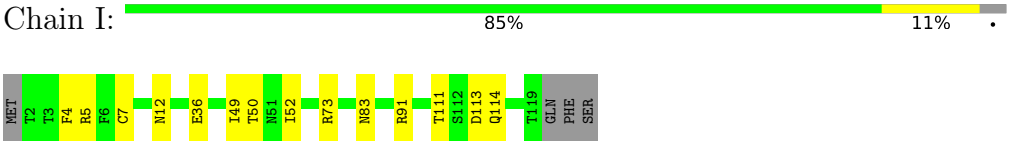
• Molecule 9: DNA-directed RNA polymerases I, II, and III subunit RPABC3

Chain H:



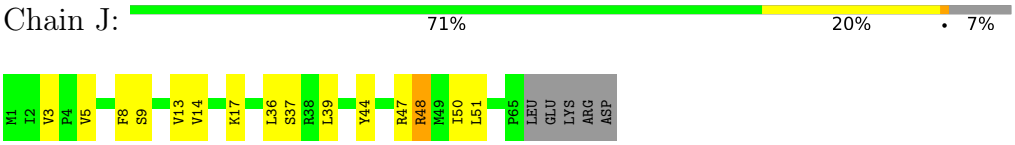
• Molecule 10: DNA-directed RNA polymerase II subunit RPB9

Chain I:



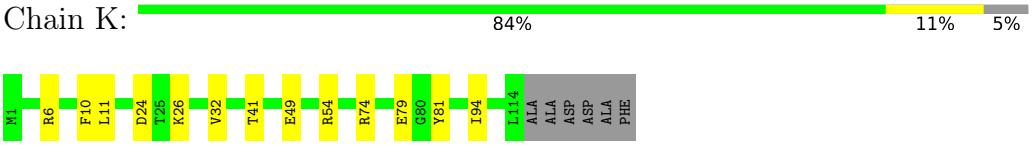
• Molecule 11: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



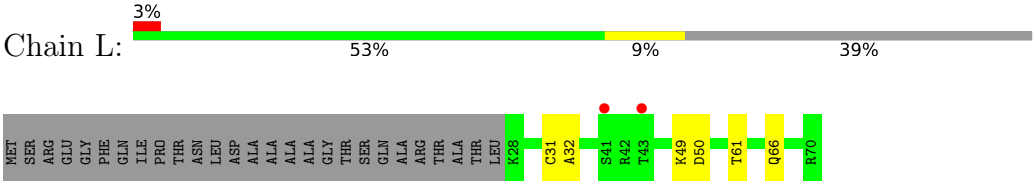
• Molecule 12: DNA-directed RNA polymerase II subunit RPB11

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	167.66Å 222.90Å 193.49Å 90.00° 100.85° 90.00°	Depositor
Resolution (Å)	49.04 – 3.10 49.04 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.04-3.10) 100.0 (49.04-3.10)	Depositor EDS
R_{merge}	0.36	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.224 , 0.269 0.224 , 0.269	Depositor DCC
R_{free} test set	1849 reflections (1.47%)	wwPDB-VP
Wilson B-factor (Å^2)	64.3	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 49.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29075	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PPV, MG, G35, ZN

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	0.72	1/248 (0.4%)	0.79	0/384
2	T	0.63	0/551	1.06	0/843
3	N	0.65	0/359	0.84	0/553
4	A	0.28	0/11012	0.49	2/14895 (0.0%)
5	B	0.29	0/9030	0.48	0/12186
6	C	0.30	0/2139	0.49	0/2899
7	E	0.27	0/1767	0.48	0/2378
8	F	0.27	0/696	0.47	0/943
9	H	0.27	0/1082	0.51	0/1466
10	I	0.30	0/970	0.50	0/1308
11	J	0.29	0/541	0.48	0/727
12	K	0.28	0/937	0.48	0/1265
13	L	0.34	0/339	0.52	0/450
All	All	0.31	1/29671 (0.0%)	0.52	2/40297 (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	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	1	A	OP3-P	-10.56	1.48	1.61

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	398	GLU	C-N-CA	6.14	137.05	121.70
4	A	266	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	1311	VAL	Peptide
4	A	311	GLN	Peptide
4	A	524	VAL	Peptide
4	A	53	LEU	Peptide
4	A	55	ASP	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	221	0	110	3	0
2	T	520	0	299	8	0
3	N	317	0	166	2	0
4	A	10820	0	10862	156	0
5	B	8859	0	8816	138	0
6	C	2101	0	2056	29	0
7	E	1731	0	1758	22	0
8	F	684	0	692	13	0
9	H	1064	0	1029	17	0
10	I	952	0	899	9	0
11	J	532	0	542	10	0
12	K	919	0	929	15	0
13	L	337	0	352	5	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	9	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	29075	0	28510	370	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 6.

All (370) 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)
5:B:213:ILE:O	5:B:215:GLN:NE2	1.90	1.02
2:T:19:G35:H1'	4:A:835:GLY:HA3	1.62	0.81
5:B:999:MET:HE2	5:B:1000:PRO:HD2	1.63	0.81
4:A:262:LEU:O	4:A:266:LEU:HD23	1.86	0.76
6:C:66:ARG:NH2	11:J:3:VAL:O	2.21	0.74
5:B:29:ASP:HB3	5:B:658:ILE:HG12	1.71	0.73
12:K:10:PHE:CE2	12:K:11:LEU:HD13	2.23	0.72
4:A:471:ASN:O	4:A:474:VAL:HG12	1.89	0.72
5:B:843:GLN:HG2	5:B:993:THR:HB	1.70	0.72
9:H:37:LYS:H	9:H:126:GLU:HB2	1.53	0.71
7:E:127:ILE:HG22	7:E:129:PRO:HD2	1.73	0.70
9:H:105:GLU:HB3	9:H:113:ALA:HB3	1.74	0.69
5:B:128:LEU:HD11	5:B:170:LEU:HB3	1.74	0.69
5:B:763:GLN:HG2	5:B:766:ARG:HG2	1.73	0.68
12:K:10:PHE:CD2	12:K:11:LEU:CD1	2.76	0.68
6:C:165:LYS:O	12:K:6:ARG:NH1	2.27	0.68
4:A:875:ALA:HB2	4:A:1366:ARG:HD2	1.77	0.67
5:B:763:GLN:HG3	5:B:765:PRO:HD2	1.76	0.67
5:B:995:ARG:NH1	5:B:997:GLU:OE1	2.28	0.67
9:H:5:LEU:HD12	9:H:134:ASN:H	1.60	0.66
5:B:639:ILE:HD11	5:B:691:GLU:HB2	1.78	0.65
5:B:999:MET:HE3	5:B:999:MET:HA	1.79	0.65
5:B:998:ASP:OD1	6:C:35:ARG:NH2	2.29	0.64
5:B:884:ARG:HH11	5:B:935:ARG:HD3	1.61	0.64
5:B:1056:SER:HB3	5:B:1066:SER:HB2	1.80	0.63
2:T:19:G35:H4	4:A:832:ALA:HA	1.79	0.63
5:B:793:ALA:HB3	5:B:856:PHE:HB2	1.80	0.63
4:A:329:LEU:HA	4:A:335:ARG:H	1.63	0.63
4:A:740:LEU:HD12	6:C:192:TRP:CD1	2.34	0.63
4:A:1311:VAL:O	4:A:1312:ASN:ND2	2.21	0.62
6:C:142:VAL:HG11	11:J:5:VAL:HG13	1.80	0.62
4:A:900:ASP:HA	4:A:926:GLN:HE22	1.64	0.62
5:B:205:ILE:HG13	5:B:461:LEU:HB3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:897:TYR:HD2	4:A:936:LEU:HD13	1.63	0.62
5:B:629:ASP:O	5:B:632:ARG:NH1	2.33	0.62
11:J:14:VAL:HB	11:J:50:ILE:HD11	1.82	0.61
4:A:1135:ARG:NH1	4:A:1284:MET:SD	2.74	0.61
4:A:1325:THR:OG1	7:E:146:HIS:O	2.17	0.61
4:A:1329:THR:HG22	4:A:1331:SER:H	1.64	0.61
4:A:134:ARG:NH2	4:A:220:THR:O	2.32	0.61
5:B:416:LEU:HD23	5:B:457:LEU:HD23	1.82	0.60
12:K:10:PHE:CE2	12:K:11:LEU:CD1	2.84	0.60
5:B:1135:ARG:NH2	5:B:1136:ASP:OD1	2.34	0.60
4:A:208:LEU:HD23	4:A:235:ILE:HD11	1.83	0.60
5:B:325:GLN:OE1	10:I:12:ASN:ND2	2.35	0.60
4:A:1265:ASN:ND2	5:B:263:GLY:O	2.35	0.60
5:B:612:GLU:O	5:B:632:ARG:NH2	2.31	0.60
1:R:9:G:H1	2:T:20:DC:H42	1.48	0.59
5:B:229:ALA:O	5:B:261:ARG:NH2	2.34	0.59
11:J:36:LEU:HD11	11:J:51:LEU:HB2	1.84	0.59
4:A:54:ASN:HB2	4:A:244:PRO:HG3	1.83	0.59
6:C:35:ARG:NH1	12:K:41:THR:OG1	2.35	0.59
4:A:326:ARG:HG2	4:A:1406:VAL:HG11	1.82	0.59
4:A:535:THR:HG21	4:A:617:VAL:HG23	1.84	0.59
5:B:863:GLU:O	5:B:961:LEU:HD22	2.03	0.59
4:A:378:GLU:OE2	4:A:387:ARG:NH2	2.36	0.59
4:A:1107:VAL:HG22	4:A:1383:SER:HB3	1.84	0.59
12:K:24:ASP:OD2	12:K:74:ARG:NH1	2.35	0.59
4:A:549:MET:HG2	4:A:652:VAL:HG13	1.84	0.59
11:J:37:SER:OG	11:J:47:ARG:NH2	2.35	0.59
4:A:1399:ARG:HB3	4:A:1408:ILE:HD13	1.83	0.58
11:J:9:SER:OG	11:J:48:ARG:NH2	2.37	0.58
6:C:66:ARG:NH1	6:C:144:ILE:O	2.37	0.58
4:A:108:MET:SD	4:A:171:GLN:NE2	2.76	0.58
2:T:19:G35:H3'	2:T:19:G35:HN3	1.68	0.58
5:B:862:GLN:OE1	5:B:957:ASN:ND2	2.37	0.58
10:I:50:THR:HG22	10:I:52:ILE:H	1.68	0.58
4:A:707:GLY:HA3	4:A:1281:ARG:HG3	1.85	0.58
5:B:238:ALA:HB3	5:B:256:VAL:HB	1.86	0.58
5:B:334:ILE:HG21	5:B:352:ALA:HB2	1.85	0.57
10:I:111:THR:HG22	10:I:113:ASP:H	1.69	0.57
4:A:150:THR:HA	4:A:166:GLY:HA3	1.86	0.57
8:F:111:LEU:HD23	8:F:111:LEU:H	1.68	0.57
4:A:1129:GLU:HA	4:A:1132:LYS:HD2	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:128:LYS:HD3	8:F:149:GLU:HA	1.86	0.57
4:A:1438:THR:HG23	8:F:92:ARG:HB2	1.87	0.57
5:B:29:ASP:OD2	5:B:655:LYS:NZ	2.36	0.57
4:A:338:GLY:HA2	5:B:1129:ARG:HH22	1.68	0.57
4:A:824:LEU:HD21	5:B:765:PRO:HB3	1.87	0.57
6:C:93:ASP:O	6:C:127:ARG:NH2	2.37	0.56
4:A:535:THR:O	4:A:575:LYS:NZ	2.38	0.56
9:H:94:ASP:OD1	9:H:94:ASP:N	2.39	0.56
2:T:25:DC:OP1	5:B:857:ARG:NH2	2.39	0.56
5:B:847:ASP:OD2	12:K:6:ARG:NH2	2.39	0.56
4:A:890:ASP:OD1	4:A:940:ARG:NH1	2.38	0.56
4:A:666:ILE:HG23	5:B:1026:LEU:HB2	1.86	0.56
4:A:806:ARG:NH2	5:B:725:PRO:O	2.39	0.56
5:B:103:ASN:OD1	5:B:169:ARG:NH2	2.38	0.56
5:B:287:ARG:NH1	5:B:324:ILE:O	2.39	0.56
11:J:17:LYS:HB3	11:J:39:LEU:HD13	1.88	0.56
5:B:904:ARG:NH1	13:L:66:GLN:O	2.39	0.56
4:A:72:GLU:HB3	4:A:76:GLU:HB3	1.87	0.55
4:A:945:GLU:O	7:E:201:LYS:NZ	2.39	0.55
9:H:28:ALA:HB3	9:H:38:LEU:HB3	1.87	0.55
4:A:870:GLU:O	7:E:205:SER:OG	2.20	0.55
5:B:269:ILE:HD11	5:B:386:LEU:HD21	1.87	0.55
7:E:88:VAL:HG23	7:E:92:THR:HB	1.88	0.55
4:A:1161:THR:HG21	4:A:1166:ASP:HB2	1.89	0.55
4:A:523:ILE:HG23	4:A:527:THR:HB	1.89	0.55
5:B:217:ARG:NH1	5:B:407:ASP:OD1	2.40	0.55
4:A:4:GLN:NE2	4:A:76:GLU:OE2	2.40	0.55
4:A:76:GLU:OE2	5:B:1159:ARG:NH1	2.40	0.55
5:B:260:GLY:O	5:B:267:ARG:NH1	2.38	0.55
4:A:243:PRO:HB2	4:A:245:PRO:HD2	1.89	0.55
4:A:463:ILE:HD12	4:A:465:TYR:H	1.72	0.55
4:A:913:LEU:HD22	4:A:915:SER:H	1.72	0.55
4:A:1106:ASN:ND2	4:A:1385:THR:OG1	2.40	0.55
9:H:39:THR:HB	9:H:124:ARG:HB3	1.89	0.55
12:K:10:PHE:CD2	12:K:11:LEU:HD12	2.42	0.54
5:B:884:ARG:HE	5:B:935:ARG:HH21	1.54	0.54
4:A:579:SER:HB3	4:A:611:GLN:HA	1.90	0.54
12:K:10:PHE:CD2	12:K:11:LEU:HD13	2.40	0.54
4:A:666:ILE:HD12	4:A:667:GLY:N	2.23	0.54
5:B:653:VAL:HG22	5:B:689:LEU:HB3	1.90	0.54
5:B:999:MET:HA	5:B:999:MET:CE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:738:LYS:HD2	4:A:740:LEU:HD21	1.90	0.53
5:B:208:SER:OG	5:B:210:LYS:NZ	2.41	0.53
4:A:491:VAL:O	5:B:1150:ARG:NH2	2.42	0.53
5:B:979:LYS:HE2	5:B:1095:LEU:HD12	1.91	0.53
4:A:170:THR:O	4:A:185:TRP:NE1	2.33	0.53
4:A:795:GLU:HG2	5:B:731:VAL:HG11	1.90	0.53
9:H:116:TYR:HB2	9:H:123:MET:HB3	1.90	0.53
10:I:5:ARG:NH2	10:I:36:GLU:OE2	2.42	0.53
12:K:10:PHE:HD2	12:K:11:LEU:HD12	1.74	0.53
11:J:44:TYR:HA	11:J:47:ARG:HB2	1.91	0.53
4:A:5:GLN:O	5:B:1159:ARG:NH2	2.38	0.52
4:A:1113:THR:O	4:A:1330:ASN:ND2	2.41	0.52
5:B:1103:ILE:O	5:B:1122:ARG:NH1	2.42	0.52
6:C:177:GLU:HB2	6:C:231:ASN:HB3	1.91	0.52
4:A:997:LEU:O	4:A:1011:GLN:NE2	2.42	0.52
4:A:443:LEU:HD21	4:A:455:MET:HB3	1.91	0.52
4:A:679:ILE:HG23	4:A:729:ALA:HB1	1.92	0.52
5:B:1106:ARG:NH2	5:B:1111:MET:SD	2.82	0.52
9:H:80:ARG:NH2	12:K:79:GLU:OE2	2.37	0.52
6:C:2:SER:OG	6:C:3:GLU:N	2.42	0.52
5:B:1174:LYS:HB2	5:B:1179:GLN:HB2	1.92	0.51
5:B:128:LEU:HD11	5:B:170:LEU:CB	2.40	0.51
7:E:124:VAL:HG23	7:E:125:PRO:HD3	1.92	0.51
4:A:503:GLN:OE1	8:F:90:ARG:NH2	2.43	0.51
4:A:348:SER:HB2	5:B:1128:LEU:HB2	1.93	0.51
5:B:837:ASP:OD2	5:B:1020:ARG:NH2	2.43	0.51
4:A:78:PRO:O	5:B:1205:GLN:NE2	2.40	0.51
4:A:607:ILE:HG12	4:A:612:ILE:HG22	1.92	0.51
5:B:424:LEU:HD11	5:B:448:ILE:HG23	1.93	0.51
4:A:69:THR:O	4:A:69:THR:HG22	2.10	0.51
4:A:910:PRO:HA	4:A:916:GLY:HA3	1.93	0.51
5:B:999:MET:HG3	5:B:1000:PRO:HD2	1.93	0.51
5:B:394:ASP:OD2	10:I:91:ARG:HD2	2.11	0.50
4:A:42:ASP:HA	4:A:50:ILE:HB	1.94	0.50
4:A:457:ALA:HB2	4:A:501:LEU:HD12	1.93	0.50
5:B:610:ASN:HB3	5:B:613:VAL:HG23	1.93	0.50
4:A:846:GLU:HA	4:A:1066:VAL:HG22	1.93	0.50
4:A:871:ASP:OD1	4:A:1366:ARG:NH2	2.42	0.50
1:R:7:A:H2'	1:R:8:G:H8	1.77	0.50
10:I:73:ARG:O	10:I:83:ASN:ND2	2.44	0.50
4:A:434:ARG:NH2	4:A:440:ASP:OD2	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:446:ARG:NH1	4:A:447:GLN:O	2.45	0.50
4:A:715:GLU:OE2	4:A:774:ARG:NH1	2.41	0.49
2:T:17:DG:OP1	4:A:326:ARG:NH2	2.46	0.49
5:B:788:ARG:NH1	5:B:790:ASP:OD1	2.45	0.49
6:C:6:PRO:HB3	6:C:25:VAL:HG22	1.94	0.49
5:B:835:GLN:HA	5:B:1013:ASN:HD22	1.78	0.49
5:B:287:ARG:NH2	5:B:294:ASP:OD1	2.45	0.49
7:E:39:LEU:HG	7:E:43:LYS:HE2	1.94	0.49
4:A:43:GLU:O	4:A:46:THR:OG1	2.29	0.49
4:A:269:ILE:HG22	4:A:299:HIS:HB3	1.94	0.49
4:A:115:LEU:HD23	4:A:142:CYS:HB3	1.95	0.48
4:A:881:GLN:NE2	4:A:958:VAL:O	2.40	0.48
5:B:549:THR:HB	5:B:628:THR:HB	1.94	0.48
9:H:12:VAL:HA	9:H:28:ALA:HA	1.95	0.48
4:A:18:GLN:NE2	4:A:19:PHE:O	2.46	0.48
4:A:146:MET:O	4:A:171:GLN:N	2.39	0.48
6:C:54:ASN:ND2	6:C:60:ASP:OD1	2.46	0.48
4:A:1142:THR:O	4:A:1145:SER:OG	2.31	0.48
4:A:768:GLN:HG2	4:A:816:HIS:HA	1.94	0.48
4:A:1118:VAL:HB	4:A:1306:LEU:HB2	1.95	0.48
5:B:863:GLU:O	5:B:961:LEU:CD2	2.61	0.48
5:B:890:TYR:OH	5:B:936:ASP:OD2	2.32	0.48
4:A:388:LEU:HD13	4:A:432:VAL:HB	1.95	0.48
5:B:847:ASP:HB3	6:C:167:HIS:CE1	2.48	0.48
7:E:59:SER:HB3	7:E:81:GLU:HA	1.96	0.48
12:K:49:GLU:HG3	12:K:94:ILE:HG13	1.95	0.48
5:B:356:LEU:HA	5:B:360:PHE:HB3	1.96	0.47
5:B:1193:GLN:HE21	5:B:1195:HIS:HE1	1.62	0.47
1:R:5:A:H2'	1:R:6:G:H8	1.78	0.47
5:B:96:TYR:HB2	5:B:129:PHE:HB2	1.96	0.47
5:B:415:GLN:OE1	5:B:476:ARG:NH2	2.47	0.47
5:B:806:THR:HG22	5:B:808:ALA:H	1.80	0.47
7:E:24:LYS:NZ	7:E:32:GLN:OE1	2.42	0.47
8:F:76:LYS:HG3	8:F:79:ARG:HH21	1.78	0.47
4:A:100:LYS:HB3	4:A:100:LYS:HE3	1.70	0.47
4:A:666:ILE:HG23	5:B:1026:LEU:CB	2.45	0.47
5:B:114:PRO:HG2	5:B:181:LEU:HD11	1.96	0.47
5:B:218:SER:O	5:B:241:ARG:NH2	2.42	0.47
4:A:808:LEU:O	5:B:728:ARG:NH1	2.48	0.47
5:B:900:ALA:HB3	13:L:61:THR:HG23	1.96	0.47
6:C:36:VAL:HG23	6:C:40:GLU:HB2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:77:ILE:HG13	6:C:161:LYS:HE3	1.96	0.47
5:B:493:SER:OG	5:B:497:ARG:NH2	2.43	0.47
7:E:127:ILE:HB	7:E:130:ALA:HB3	1.97	0.47
9:H:145:ARG:HG2	9:H:146:ARG:HD2	1.97	0.47
4:A:517:ASN:OD1	4:A:1364:ASN:ND2	2.48	0.46
4:A:1345:ARG:NH1	4:A:1373:ASP:OD1	2.42	0.46
5:B:227:LYS:N	5:B:395:GLN:OE1	2.47	0.46
5:B:294:ASP:HB2	10:I:12:ASN:HA	1.97	0.46
9:H:30:SER:HG	9:H:36:CYS:HG	1.60	0.46
4:A:340:LEU:HD13	4:A:1429:ILE:HG13	1.97	0.46
4:A:1318:THR:HG22	7:E:142:VAL:HG22	1.96	0.46
5:B:721:LEU:HB3	5:B:722:ASP:H	1.51	0.46
6:C:179:GLU:OE1	6:C:206:ASN:ND2	2.46	0.46
4:A:761:MET:HG3	5:B:1021:MET:HG2	1.98	0.46
4:A:961:ARG:HH11	4:A:1025:ARG:HH22	1.62	0.46
5:B:760:ASP:OD1	5:B:760:ASP:N	2.40	0.46
5:B:848:ARG:NH1	11:J:8:PHE:O	2.49	0.46
4:A:50:ILE:HG23	4:A:52:GLY:H	1.80	0.46
5:B:840:ILE:HG12	5:B:992:ILE:HG22	1.97	0.46
5:B:996:ARG:NH2	6:C:174:ALA:O	2.49	0.46
8:F:85:MET:HG3	8:F:89:GLU:HG3	1.98	0.46
5:B:112:LEU:HD21	5:B:117:ALA:HB2	1.97	0.46
5:B:912:ILE:HB	5:B:939:THR:HB	1.98	0.46
7:E:64:PRO:HD3	7:E:76:GLY:HA2	1.96	0.46
4:A:179:LEU:HB3	4:A:297:GLN:HE21	1.80	0.46
4:A:660:ASN:O	5:B:1082:MET:N	2.49	0.46
4:A:1343:ALA:HB2	7:E:150:VAL:HG22	1.98	0.46
5:B:830:TYR:CZ	5:B:1000:PRO:HD3	2.51	0.46
4:A:346:ASP:HB3	5:B:1108:ARG:H	1.81	0.46
4:A:896:ARG:HH12	4:A:1030:ARG:HH21	1.63	0.46
5:B:185:THR:OG1	5:B:188:ASP:OD1	2.33	0.46
5:B:211:VAL:HG13	5:B:495:LEU:HD23	1.97	0.46
5:B:901:PRO:HA	5:B:949:VAL:HB	1.98	0.46
4:A:38:PRO:HG3	4:A:271:LYS:HG2	1.99	0.45
4:A:90:VAL:HG23	4:A:236:LEU:HB2	1.98	0.45
4:A:1345:ARG:HG2	4:A:1372:VAL:HG12	1.98	0.45
8:F:128:LYS:NZ	8:F:148:VAL:O	2.38	0.45
4:A:550:LEU:HG	4:A:556:TRP:CE2	2.51	0.45
4:A:1303:GLU:OE1	4:A:1326:ARG:NH1	2.49	0.45
4:A:452:LYS:O	5:B:1141:HIS:NE2	2.47	0.45
5:B:864:LYS:HA	5:B:961:LEU:HD22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:46:ILE:HA	6:C:159:ALA:HA	1.99	0.45
4:A:1356:ILE:HG21	4:A:1363:VAL:HG23	1.99	0.45
5:B:293:PRO:HG2	5:B:296:GLU:HB2	1.98	0.45
4:A:380:VAL:HG12	4:A:388:LEU:HD12	1.99	0.45
4:A:853:ASP:OD1	4:A:855:THR:OG1	2.30	0.45
4:A:1062:GLU:HG2	8:F:88:TYR:HE2	1.81	0.45
5:B:577:ALA:HB1	5:B:589:VAL:HG13	1.98	0.45
9:H:62:SER:OG	9:H:63:LEU:N	2.50	0.45
5:B:102:VAL:HG22	5:B:112:LEU:HB2	1.98	0.45
5:B:518:HIS:HB3	5:B:522:VAL:HG12	1.99	0.45
4:A:443:LEU:HD12	4:A:501:LEU:HD11	1.99	0.44
4:A:451:HIS:CE1	4:A:1074:GLU:CD	2.91	0.44
5:B:1002:THR:HG23	5:B:1004:GLU:H	1.81	0.44
4:A:260:ASP:OD1	4:A:261:ASP:N	2.48	0.44
7:E:55:ARG:NH2	7:E:137:GLU:OE1	2.50	0.44
4:A:230:ARG:HG3	4:A:232:GLU:HG2	1.99	0.44
4:A:781:ASP:HB2	4:A:789:LYS:HD3	1.99	0.44
5:B:384:ARG:HA	5:B:384:ARG:HD3	1.74	0.44
5:B:103:ASN:ND2	5:B:109:THR:OG1	2.50	0.44
5:B:1135:ARG:HG3	5:B:1147:LEU:HD21	2.00	0.44
4:A:336:ILE:HD13	4:A:340:LEU:HD12	2.00	0.44
5:B:281:PRO:HD2	5:B:284:ILE:HD12	1.99	0.44
6:C:10:ILE:HD13	6:C:20:PHE:HB3	2.00	0.44
7:E:135:PHE:HB3	7:E:140:LEU:HD11	1.99	0.44
4:A:344:ARG:NH1	5:B:1127:GLY:O	2.44	0.44
4:A:1025:ARG:HE	4:A:1030:ARG:HH12	1.65	0.44
5:B:46:GLN:H	5:B:46:GLN:HG3	1.63	0.44
4:A:108:MET:SD	4:A:108:MET:N	2.90	0.44
4:A:362:ASP:HB3	4:A:508:PRO:HD3	2.00	0.44
4:A:1428:VAL:HG13	5:B:1151:LEU:HD21	1.98	0.44
4:A:575:LYS:O	4:A:579:SER:OG	2.35	0.43
4:A:956:LEU:HD13	4:A:1021:LEU:HD22	2.00	0.43
5:B:1101:ASP:O	5:B:1122:ARG:NE	2.47	0.43
7:E:147:HIS:HB3	7:E:150:VAL:HG23	2.00	0.43
4:A:1328:TYR:OH	4:A:1351:GLU:OE1	2.33	0.43
5:B:273:LEU:HB2	5:B:276:ILE:HB	1.99	0.43
5:B:326:ASP:OD1	5:B:326:ASP:N	2.51	0.43
5:B:1099:VAL:HG12	5:B:1103:ILE:HD11	1.99	0.43
4:A:436:ILE:HD11	4:A:491:VAL:HG11	1.99	0.43
4:A:1276:VAL:HB	4:A:1279:ILE:HD13	2.00	0.43
5:B:245:GLU:OE1	5:B:246:LYS:NZ	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:644:LYS:HB2	4:A:644:LYS:HE3	1.88	0.43
5:B:834:ASN:HB3	5:B:840:ILE:HG13	2.00	0.43
4:A:1148:ILE:HG12	10:I:49:ILE:HD12	2.00	0.43
4:A:24:PRO:HB3	4:A:238:CYS:HB3	2.01	0.43
5:B:1100:ASP:HA	5:B:1103:ILE:HG12	2.01	0.43
4:A:1335:ILE:HG23	4:A:1339:LEU:HD12	2.00	0.43
12:K:32:VAL:HG22	12:K:74:ARG:HG3	2.00	0.43
4:A:351:THR:OG1	4:A:352:VAL:N	2.52	0.43
5:B:744:HIS:ND1	5:B:746:SER:OG	2.36	0.43
5:B:805:THR:HG21	5:B:815:ARG:HD3	2.01	0.43
7:E:197:LYS:HE2	7:E:199:ILE:HD11	2.01	0.43
4:A:884:ASP:OD1	4:A:896:ARG:NH2	2.45	0.42
4:A:1281:ARG:HB3	4:A:1309:ASP:HB2	2.01	0.42
5:B:104:GLU:OE1	5:B:110:HIS:NE2	2.43	0.42
8:F:79:ARG:NH2	8:F:150:GLU:OE1	2.52	0.42
12:K:54:ARG:H	12:K:54:ARG:HE	1.67	0.42
4:A:683:ILE:HG21	4:A:801:GLU:HG3	2.00	0.42
4:A:1323:ASP:OD1	4:A:1325:THR:HG22	2.19	0.42
4:A:1366:ARG:H	4:A:1366:ARG:HG2	1.62	0.42
5:B:796:LEU:HB3	5:B:799:PRO:HG3	2.00	0.42
4:A:59:GLY:HA2	4:A:67:CYS:SG	2.60	0.42
4:A:1166:ASP:HA	4:A:1169:ILE:HD13	2.02	0.42
4:A:691:LEU:HD22	4:A:695:LYS:HE2	2.00	0.42
5:B:408:LEU:HD12	5:B:408:LEU:HA	1.80	0.42
6:C:52:GLU:OE2	6:C:154:LYS:NZ	2.49	0.42
9:H:81:PRO:HA	9:H:82:PRO:HD3	1.91	0.42
6:C:44:LEU:HB2	6:C:77:ILE:HD13	2.01	0.42
4:A:404:TYR:HD2	4:A:412:ARG:HB3	1.84	0.42
5:B:705:MET:HE2	5:B:745:PRO:HB3	2.02	0.42
6:C:114:TYR:CG	6:C:140:ASN:HB3	2.55	0.42
4:A:74:MET:O	5:B:1116:ARG:NH2	2.52	0.42
5:B:977:GLY:N	5:B:990:ILE:O	2.53	0.42
6:C:40:GLU:OE1	6:C:254:LYS:NZ	2.37	0.42
8:F:77:ASP:OD1	8:F:77:ASP:N	2.43	0.42
13:L:50:ASP:OD1	13:L:50:ASP:N	2.53	0.42
2:T:10:DT:O2	3:N:10:DG:N2	2.53	0.42
5:B:778:MET:SD	5:B:794:ASN:HB3	2.60	0.42
7:E:116:ILE:HG23	7:E:120:ALA:HB3	2.02	0.42
4:A:1398:MET:N	4:A:1426:GLU:OE2	2.52	0.42
5:B:383:ASN:OD1	5:B:384:ARG:NH1	2.53	0.42
5:B:615:MET:HG2	5:B:626:ILE:HG23	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:93:ILE:HD13	8:F:93:ILE:HA	1.93	0.42
4:A:1118:VAL:HA	4:A:1327:ILE:HD12	2.02	0.41
6:C:41:ILE:HA	6:C:42:PRO:HD3	1.86	0.41
8:F:97:ARG:HD2	8:F:97:ARG:HA	1.74	0.41
13:L:49:LYS:HE2	13:L:49:LYS:HB3	1.87	0.41
3:N:11:DA:H2"	3:N:12:DG:C8	2.54	0.41
5:B:487:THR:H	5:B:490:SER:HB3	1.84	0.41
6:C:114:TYR:HB3	6:C:141:GLY:H	1.85	0.41
7:E:100:ILE:HD13	7:E:100:ILE:HA	1.95	0.41
11:J:13:VAL:O	11:J:17:LYS:NZ	2.35	0.41
4:A:903:ASN:OD1	4:A:904:THR:N	2.53	0.41
4:A:571:LEU:HD23	9:H:46:LEU:HD11	2.02	0.41
5:B:895:ASP:N	5:B:895:ASP:OD1	2.52	0.41
4:A:979:SER:OG	4:A:980:ASP:N	2.54	0.41
4:A:1229:SER:OG	4:A:1233:ASP:OD2	2.38	0.41
6:C:62:PHE:O	6:C:66:ARG:HG3	2.20	0.41
5:B:1023:VAL:O	5:B:1027:ILE:HG13	2.20	0.41
4:A:800:VAL:HG13	4:A:812:GLU:HB3	2.02	0.41
4:A:1345:ARG:HG3	4:A:1376:THR:HG21	2.03	0.41
5:B:393:LYS:HD2	5:B:393:LYS:HA	1.75	0.41
4:A:533:LYS:HE2	4:A:533:LYS:HB3	1.86	0.41
4:A:683:ILE:HD13	4:A:725:ALA:HB1	2.02	0.41
4:A:702:LEU:HD23	4:A:702:LEU:HA	1.91	0.41
4:A:818:MET:HG3	5:B:514:LEU:HB3	2.01	0.41
5:B:31:TRP:CE3	5:B:34:ILE:HD12	2.56	0.41
6:C:256:ALA:HA	6:C:259:LEU:HD23	2.02	0.41
4:A:550:LEU:HD12	4:A:550:LEU:HA	1.94	0.41
5:B:364:ILE:HD13	5:B:585:VAL:HG13	2.03	0.41
5:B:840:ILE:HB	5:B:1011:ILE:HB	2.03	0.41
7:E:46:TYR:CZ	7:E:58:MET:HB2	2.54	0.41
9:H:35:GLN:OE1	9:H:128:ASN:ND2	2.53	0.41
4:A:949:ASP:OD1	4:A:949:ASP:N	2.43	0.40
4:A:1006:ILE:HD11	7:E:163:GLU:HG3	2.03	0.40
9:H:135:LEU:HB3	9:H:137:GLN:HG3	2.03	0.40
13:L:31:CYS:SG	13:L:32:ALA:N	2.94	0.40
2:T:27:DA:H5"	5:B:462:ALA:HB1	2.03	0.40
4:A:37:PHE:H	4:A:52:GLY:HA2	1.86	0.40
4:A:699:ALA:HB1	10:I:114:GLN:HG3	2.03	0.40
5:B:1104:HIS:NE2	5:B:1126:GLY:O	2.50	0.40
6:C:37:MET:SD	6:C:244:VAL:HG12	2.61	0.40
12:K:26:LYS:HE2	12:K:26:LYS:HB3	1.88	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:577:ALA:HB1	5:B:589:VAL:CG1	2.51	0.40
5:B:1183:LYS:HE3	5:B:1183:LYS:HB2	1.92	0.40
7:E:20:LYS:NZ	7:E:34:GLU:O	2.44	0.40
4:A:1198:ASP:HB3	4:A:1201:ALA:HB3	2.03	0.40
4:A:1199:ARG:NH1	4:A:1234:GLU:OE2	2.49	0.40
5:B:325:GLN:HE21	5:B:325:GLN:HB2	1.75	0.40
6:C:22:LEU:HG	6:C:25:VAL:HG21	2.03	0.40
4:A:1062:GLU:HG2	8:F:88:TYR:CE2	2.57	0.40
9:H:27:GLU:OE2	9:H:39:THR:OG1	2.37	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%)	1323 (97%)	44 (3%)	1 (0%)	51	83
5	B	1103/1224 (90%)	1070 (97%)	33 (3%)	0	100	100
6	C	265/318 (83%)	259 (98%)	6 (2%)	0	100	100
7	E	210/215 (98%)	202 (96%)	8 (4%)	0	100	100
8	F	84/155 (54%)	82 (98%)	2 (2%)	0	100	100
9	H	129/146 (88%)	121 (94%)	8 (6%)	0	100	100
10	I	116/122 (95%)	112 (97%)	4 (3%)	0	100	100
11	J	63/70 (90%)	63 (100%)	0	0	100	100
12	K	112/120 (93%)	109 (97%)	3 (3%)	0	100	100
13	L	41/70 (59%)	39 (95%)	2 (5%)	0	100	100
All	All	3491/4173 (84%)	3380 (97%)	110 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	55	ASP

5.3.2 Protein sidechains (i)

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	1193/1520 (78%)	1152 (97%)	41 (3%)	37	69
5	B	955/1061 (90%)	935 (98%)	20 (2%)	53	79
6	C	235/274 (86%)	232 (99%)	3 (1%)	69	87
7	E	193/197 (98%)	188 (97%)	5 (3%)	46	74
8	F	73/137 (53%)	71 (97%)	2 (3%)	44	74
9	H	116/128 (91%)	109 (94%)	7 (6%)	19	49
10	I	110/116 (95%)	108 (98%)	2 (2%)	59	82
11	J	60/65 (92%)	59 (98%)	1 (2%)	60	83
12	K	99/102 (97%)	98 (99%)	1 (1%)	76	90
13	L	37/57 (65%)	37 (100%)	0	100	100
All	All	3071/3657 (84%)	2989 (97%)	82 (3%)	44	74

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	12	ARG
4	A	22	PHE
4	A	36	ARG
4	A	47	ARG
4	A	67	CYS
4	A	70	CYS
4	A	74	MET
4	A	100	LYS
4	A	108	MET
4	A	134	ARG
4	A	175	ARG
4	A	180	LYS
4	A	185	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	A	203	SER
4	A	270	LEU
4	A	286	HIS
4	A	323	LYS
4	A	337	ARG
4	A	383	TYR
4	A	408	ASP
4	A	434	ARG
4	A	438	ASP
4	A	444	PHE
4	A	455	MET
4	A	629	LEU
4	A	740	LEU
4	A	816	HIS
4	A	821	ARG
4	A	847	ASP
4	A	909	ASP
4	A	961	ARG
4	A	979	SER
4	A	1000	LEU
4	A	1001	ARG
4	A	1004	ASN
4	A	1093	LYS
4	A	1274	ARG
4	A	1313	LEU
4	A	1391	ARG
4	A	1400	CYS
4	A	1410	PHE
5	B	46	GLN
5	B	65	GLU
5	B	188	ASP
5	B	199	MET
5	B	215	GLN
5	B	250	PHE
5	B	306	ASN
5	B	394	ASP
5	B	483	LEU
5	B	733	HIS
5	B	778	MET
5	B	864	LYS
5	B	895	ASP
5	B	934	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	B	953	LEU
5	B	996	ARG
5	B	1060	ARG
5	B	1072	MET
5	B	1082	MET
5	B	1195	HIS
6	C	14	SER
6	C	34	ARG
6	C	217	ASP
7	E	10	SER
7	E	11	ARG
7	E	93	MET
7	E	110	PHE
7	E	167	ARG
8	F	79	ARG
8	F	111	LEU
9	H	33	GLN
9	H	78	SER
9	H	111	LEU
9	H	124	ARG
9	H	131	ASN
9	H	136	LYS
9	H	146	ARG
10	I	4	PHE
10	I	7	CYS
11	J	48	ARG
12	K	81	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	390	GLN
4	A	515	GLN
4	A	1106	ASN
5	B	1015	HIS
5	B	1074	ASN
5	B	1195	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	9/10 (90%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	10	A

There are no RNA pucker outliers to report.

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

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	4.70	14 (77%)	20,33,36	2.11	4 (20%)

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	-	4/10/41/42	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	9.37	1.49	1.33
2	T	19	G35	O4'-C4'	7.75	1.62	1.45
2	T	19	G35	C3'-C4'	-7.19	1.33	1.53
2	T	19	G35	C5-N7	6.76	1.46	1.37
2	T	19	G35	C8-N9	6.26	1.46	1.37
2	T	19	G35	C8-N7	4.72	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	T	19	G35	O4'-C1'	-4.70	1.31	1.42
2	T	19	G35	C2-N12	4.18	1.49	1.32
2	T	19	G35	C4-N3	3.54	1.48	1.44
2	T	19	G35	O3'-C3'	2.92	1.49	1.43
2	T	19	G35	O8-C8	-2.67	1.18	1.23
2	T	19	G35	O5-C5	-2.53	1.18	1.23
2	T	19	G35	C1'-N9	2.53	1.49	1.45
2	T	19	G35	C2-N11	-2.32	1.25	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	19	G35	C2'-C1'-N9	-5.82	107.73	115.59
2	T	19	G35	C5-C4-N9	4.33	108.03	102.28
2	T	19	G35	O4'-C1'-N9	3.80	113.15	108.65
2	T	19	G35	O4'-C4'-C3'	-2.85	99.03	105.67

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	T	19	G35	O4'-C1'-N9-C4
2	T	19	G35	C3'-C4'-C5'-O5'
2	T	19	G35	O4'-C4'-C5'-O5'
2	T	19	G35	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	T	19	G35	3	0

5.5 Carbohydrates (i)

There are no monosaccharides 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	PPV	B	1301	-	6,8,8	0.74	0	13,13,13	1.09	1 (7%)

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	PPV	B	1301	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	B	1301	PPV	P2-OPP-P1	-2.44	124.45	132.83

There are no chirality outliers.

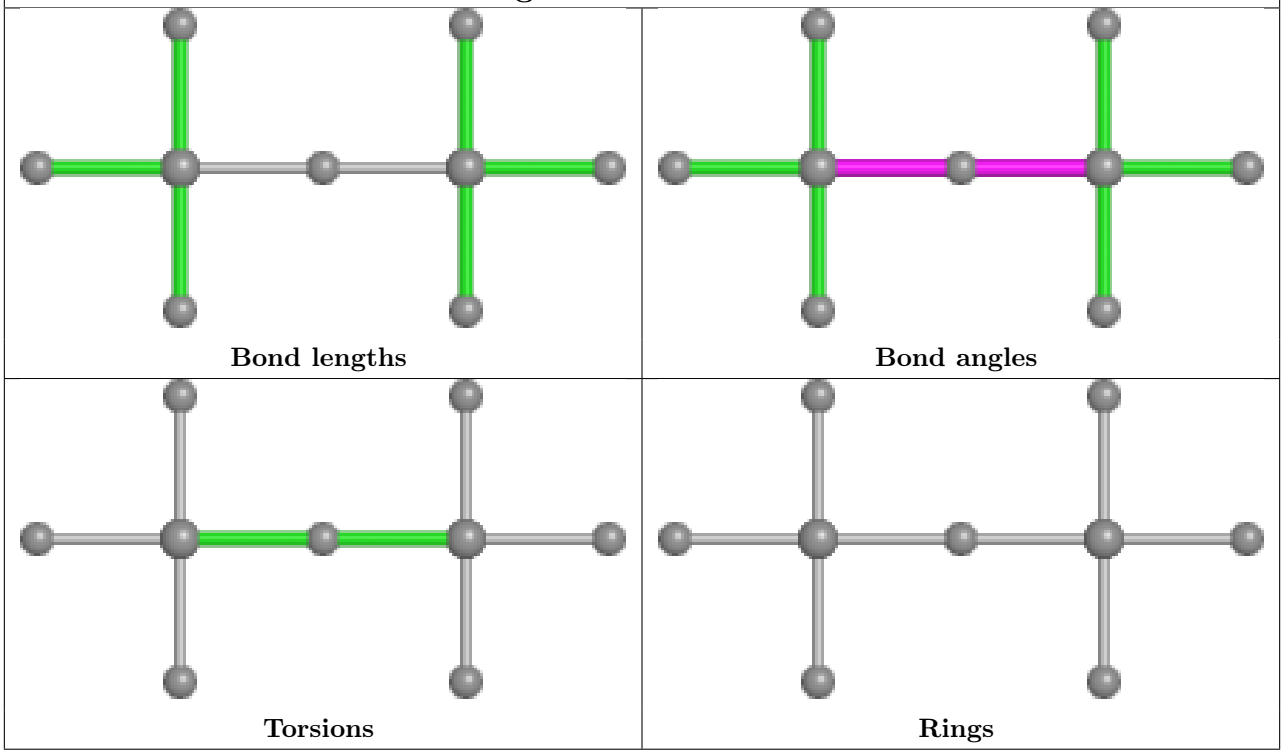
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand PPV B 1301



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

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, 95^{th} 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	10/10 (100%)	-0.39	0 100 100	94, 113, 153, 166	0
2	T	25/29 (86%)	0.42	3 (12%) 4 2	100, 180, 235, 238	0
3	N	15/18 (83%)	0.62	2 (13%) 3 1	142, 179, 248, 270	0
4	A	1382/1733 (79%)	-0.12	32 (2%) 60 39	39, 79, 157, 254	0
5	B	1123/1224 (91%)	-0.22	11 (0%) 82 67	32, 64, 125, 196	0
6	C	267/318 (83%)	-0.44	0 100 100	32, 64, 102, 141	0
7	E	212/215 (98%)	0.17	17 (8%) 12 5	55, 113, 190, 220	0
8	F	86/155 (55%)	-0.37	0 100 100	47, 78, 121, 167	0
9	H	133/146 (91%)	0.19	6 (4%) 33 16	68, 99, 149, 201	0
10	I	118/122 (96%)	-0.32	0 100 100	49, 82, 116, 170	0
11	J	65/70 (92%)	-0.45	0 100 100	37, 54, 89, 132	0
12	K	114/120 (95%)	-0.36	0 100 100	31, 67, 101, 140	0
13	L	43/70 (61%)	0.13	2 (4%) 31 15	45, 111, 159, 189	0
All	All	3593/4230 (84%)	-0.16	73 (2%) 65 44	31, 75, 156, 270	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	69	THR	8.8
4	A	44	THR	6.9
5	B	250	PHE	6.1
7	E	126	SER	5.7
7	E	91	LYS	5.6
4	A	141	LEU	5.4
4	A	45	GLN	5.1
4	A	144	THR	4.6
4	A	286	HIS	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
9	H	132	LEU	3.7
5	B	869	SER	3.6
7	E	93	MET	3.6
4	A	149	GLU	3.5
7	E	7	ARG	3.5
7	E	83	CYS	3.4
4	A	56	PRO	3.3
4	A	146	MET	3.2
4	A	111	GLY	3.2
7	E	123	LEU	3.2
5	B	106	ASP	3.1
4	A	173	THR	3.1
7	E	110	PHE	2.9
4	A	199	LEU	2.9
4	A	66	LYS	2.9
4	A	183	GLY	2.9
9	H	131	ASN	2.9
7	E	57	MET	2.8
7	E	47	CYS	2.8
7	E	118	PRO	2.8
7	E	119	SER	2.8
4	A	105	CYS	2.8
7	E	121	MET	2.7
5	B	246	LYS	2.7
9	H	84	ALA	2.7
2	T	3	DT	2.7
4	A	147	VAL	2.6
4	A	164	ARG	2.6
4	A	174	ILE	2.6
2	T	5	DC	2.6
5	B	249	ARG	2.6
4	A	1123	GLY	2.6
2	T	4	DT	2.6
7	E	129	PRO	2.6
9	H	86	ASP	2.5
9	H	139	ASN	2.5
13	L	43	THR	2.5
4	A	258	GLY	2.5
5	B	866	TYR	2.5
4	A	114	LEU	2.5
4	A	182	VAL	2.5
13	L	41	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	A	167	CYS	2.4
4	A	112	LYS	2.4
7	E	94	LYS	2.4
4	A	106	VAL	2.3
4	A	168	GLY	2.3
5	B	475	SER	2.3
7	E	76	GLY	2.3
4	A	257	ARG	2.2
3	N	11	DA	2.2
7	E	120	ALA	2.2
5	B	163	GLY	2.2
5	B	429	PHE	2.1
4	A	281	HIS	2.1
7	E	125	PRO	2.1
9	H	85	GLY	2.1
4	A	142	CYS	2.1
4	A	91	PHE	2.1
3	N	16	DA	2.0
5	B	73	GLN	2.0
5	B	248	SER	2.0
4	A	148	CYS	2.0
4	A	1329	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, 95^{th} 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	0.70	0.39	146,186,196,200	0

6.3 Carbohydrates (i)

There are no monosaccharides 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,

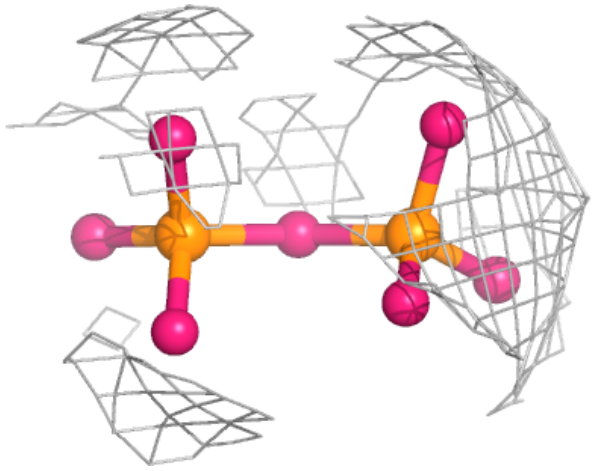
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

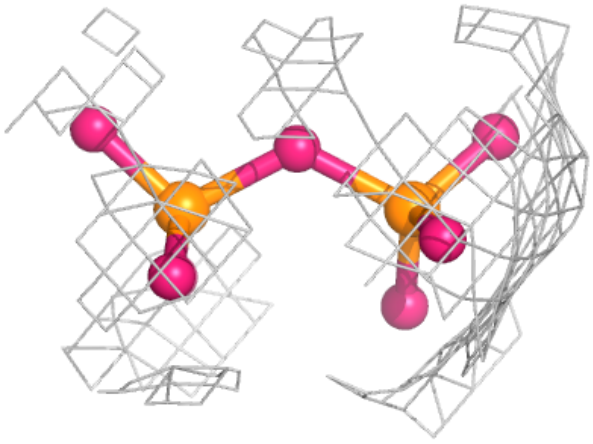
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
14	ZN	C	401	1/1	0.87	0.34	243,243,243,243	0
16	PPV	B	1301	9/9	0.89	0.26	130,140,155,155	0
14	ZN	A	1801	1/1	0.91	0.07	194,194,194,194	0
14	ZN	A	1802	1/1	0.96	0.08	105,105,105,105	0
14	ZN	L	101	1/1	0.96	0.05	137,137,137,137	0
14	ZN	B	1302	1/1	0.96	0.13	124,124,124,124	0
14	ZN	J	101	1/1	0.97	0.31	111,111,111,111	0
15	MG	A	1803	1/1	0.98	0.09	47,47,47,47	0
14	ZN	I	201	1/1	0.99	0.12	56,56,56,56	0
14	ZN	I	202	1/1	0.99	0.13	55,55,55,55	0

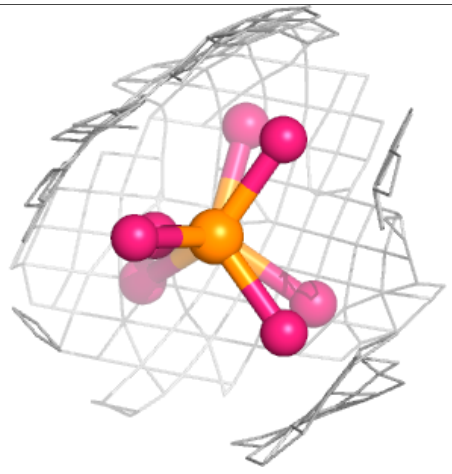
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PPV B 1301:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.