Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 11:03 pm BST

PDB ID	:	5UHC
Title	:	Crystal structure of Mycobacterium tuberculosis transcription initiation complex containing 3nt RNA in complex with Rifampin
Authors	:	Lin, W.; Das, K.; Feng, Y.; Ebright, R.H.
Deposited on	:	2017-01-11
Resolution	:	3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

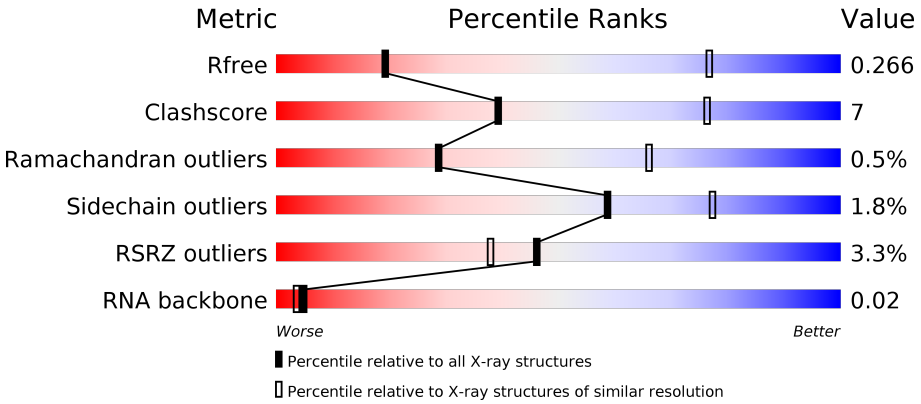
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	347	% 52% 12% 35%
1	B	347	8% 52% 13% 35%
2	C	1178	3% 77% 18%
3	D	1316	% 77% 18%

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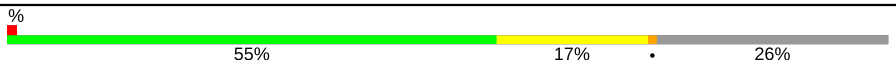
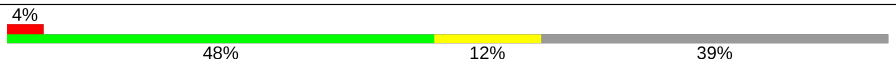
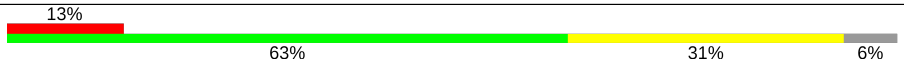
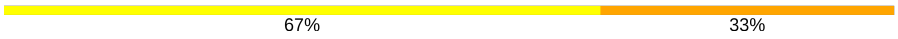
Mol	Chain	Length	Quality of chain
4	E	110	
5	F	528	
6	H	23	
7	G	16	
8	I	3	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 26105 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 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	0	0	0
			1704	1072	295	335	2			
1	B	225	Total	C	N	O	S	0	0	0
			1705	1075	289	339	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1126	Total	C	N	O	S	0	0	0
			8714	5454	1528	1693	39			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1265	Total	C	N	O	S	0	0	0
			9884	6187	1793	1864	40			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	81	Total	C	N	O	0	0	0
			637	408	106	123			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	322	Total	C	N	O	S	0	0	0
			2555	1589	461	496	9			

- Molecule 6 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP*AP*CP*GP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	23	Total	C	N	O	P	0	0	0
			476	227	91	136	22			

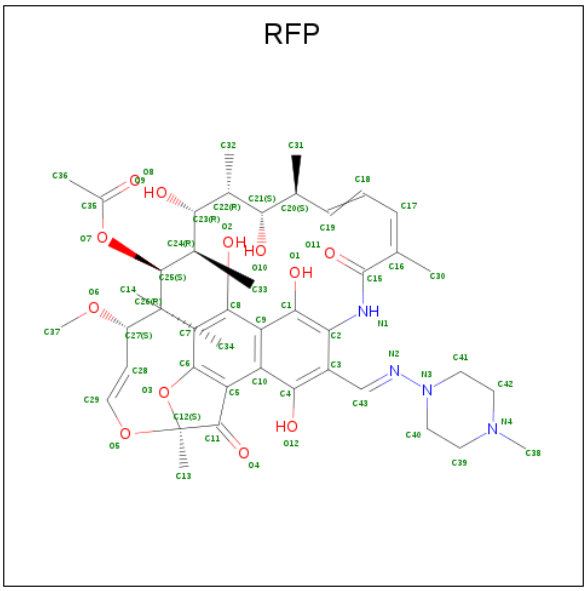
- Molecule 7 is a DNA chain called DNA (5'-D(*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	15	Total	C	N	O	P	0	0	0
			303	145	56	88	14			

- Molecule 8 is a RNA chain called RNA (5'-R(*GP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	3	Total	C	N	O	P	0	0	0
			65	30	15	18	2			

- Molecule 9 is RIFAMPICIN (three-letter code: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

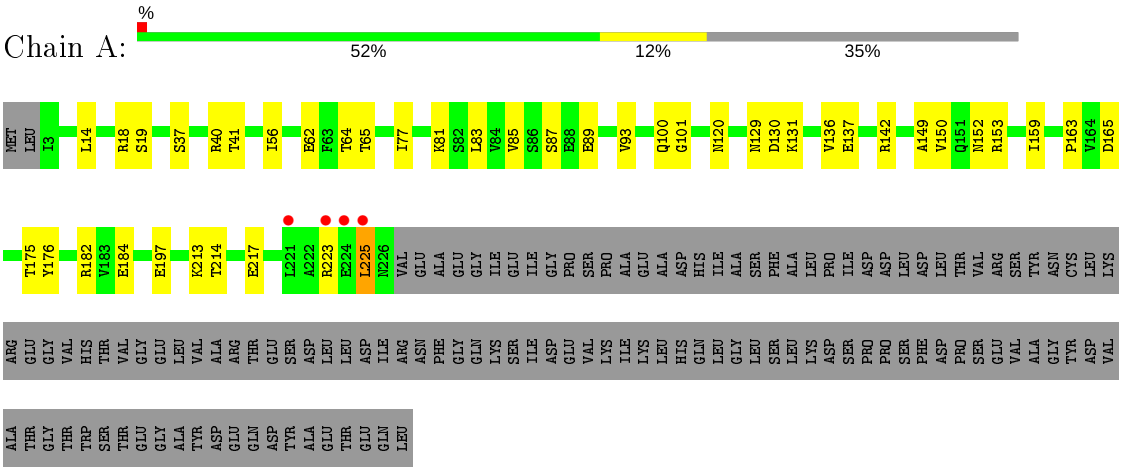
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	D	1	Total Mg 1 1	0	0

3 Residue-property plots

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

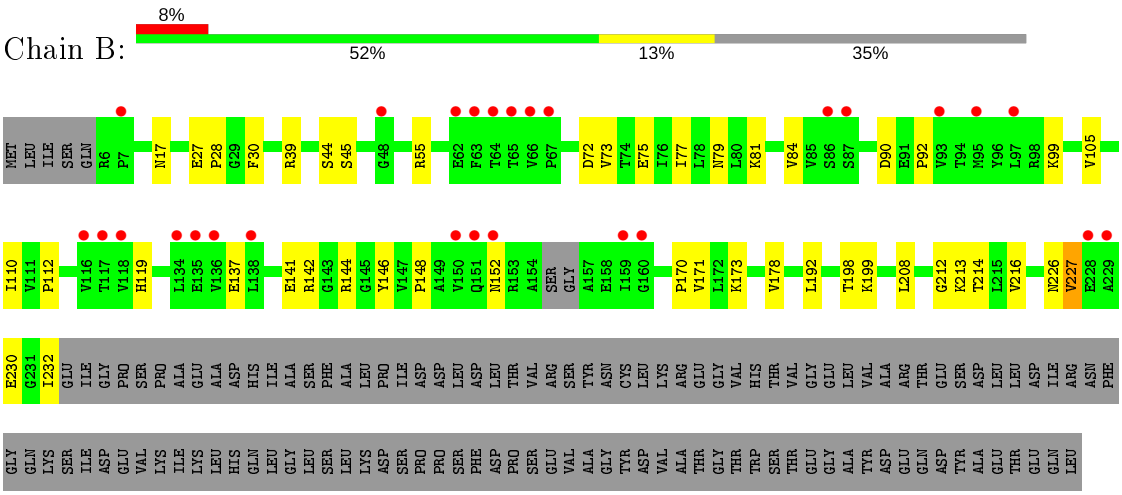
• Molecule 1: DNA-directed RNA polymerase subunit alpha

Chain A:



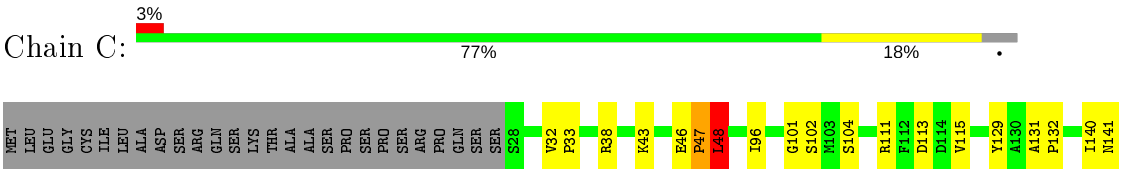
• Molecule 1: DNA-directed RNA polymerase subunit alpha

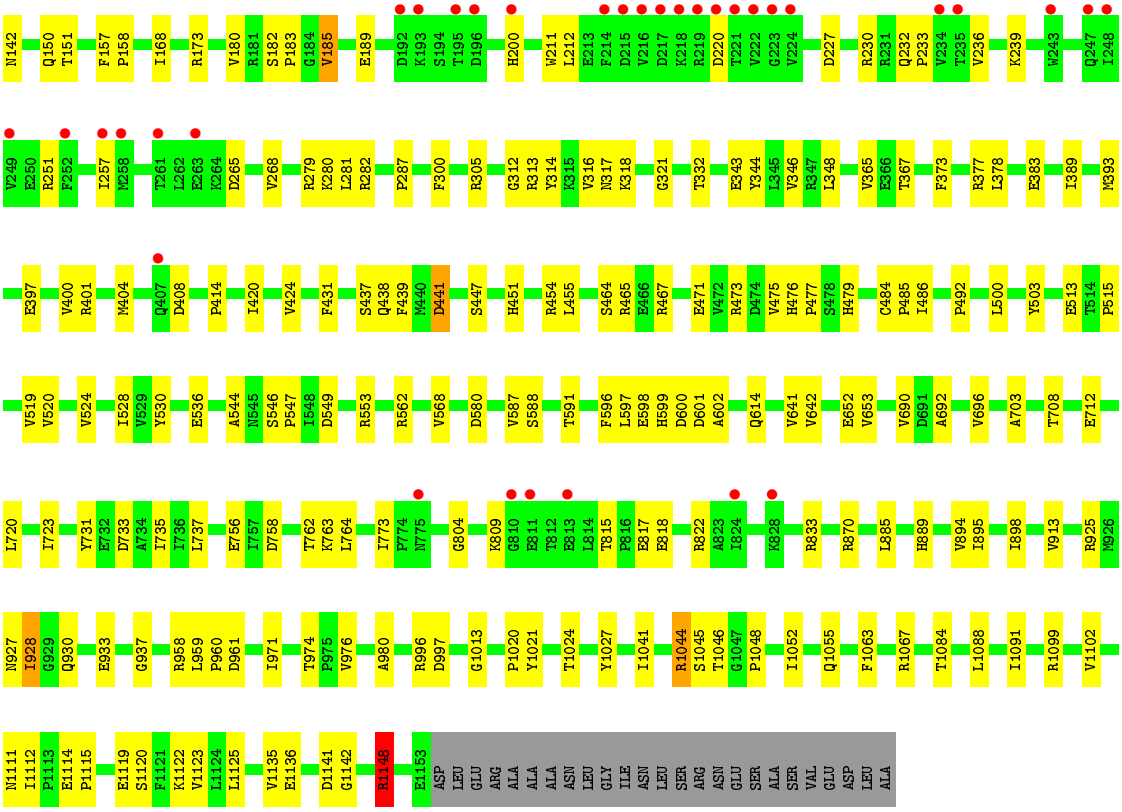
Chain B:



• Molecule 2: DNA-directed RNA polymerase subunit beta

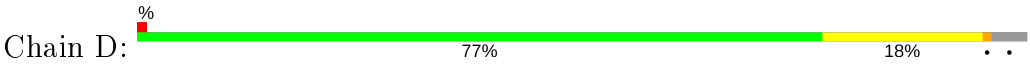
Chain C:

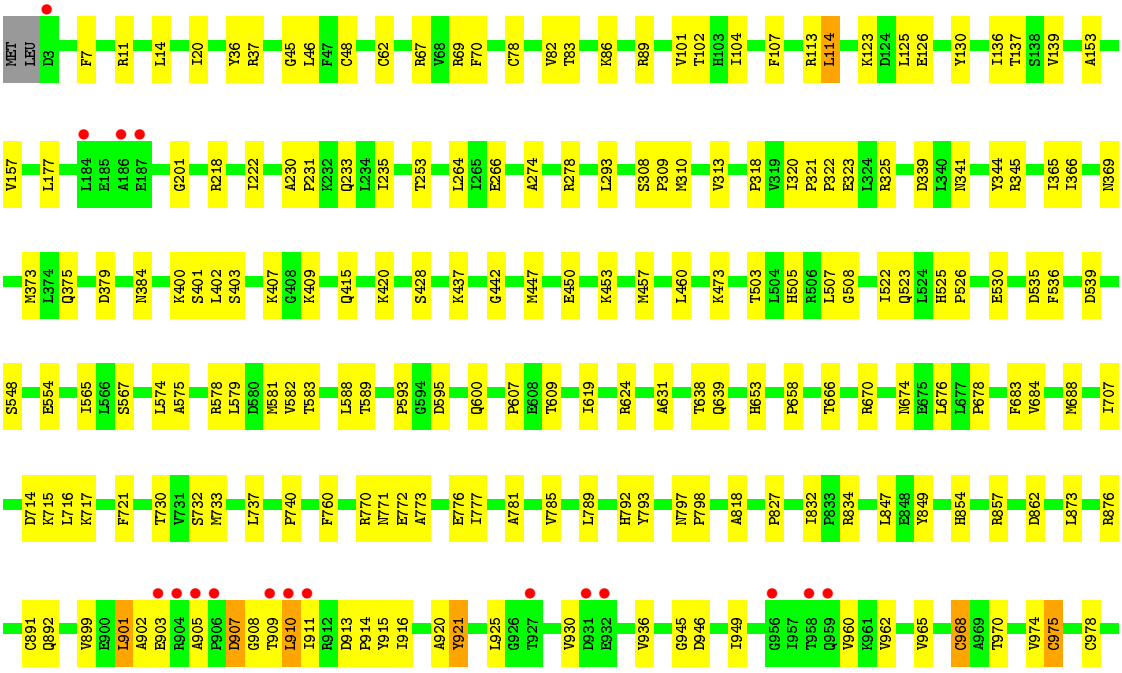


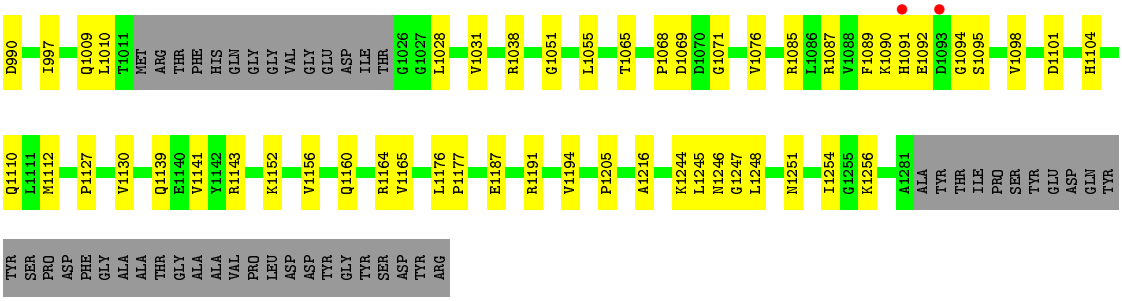


- Molecule 3: DNA-directed RNA polymerase subunit beta'

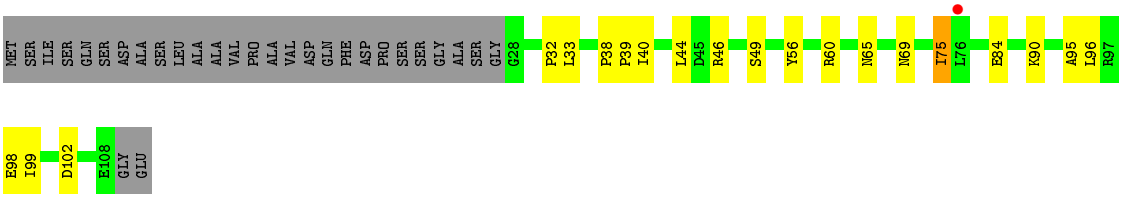
Chain D:



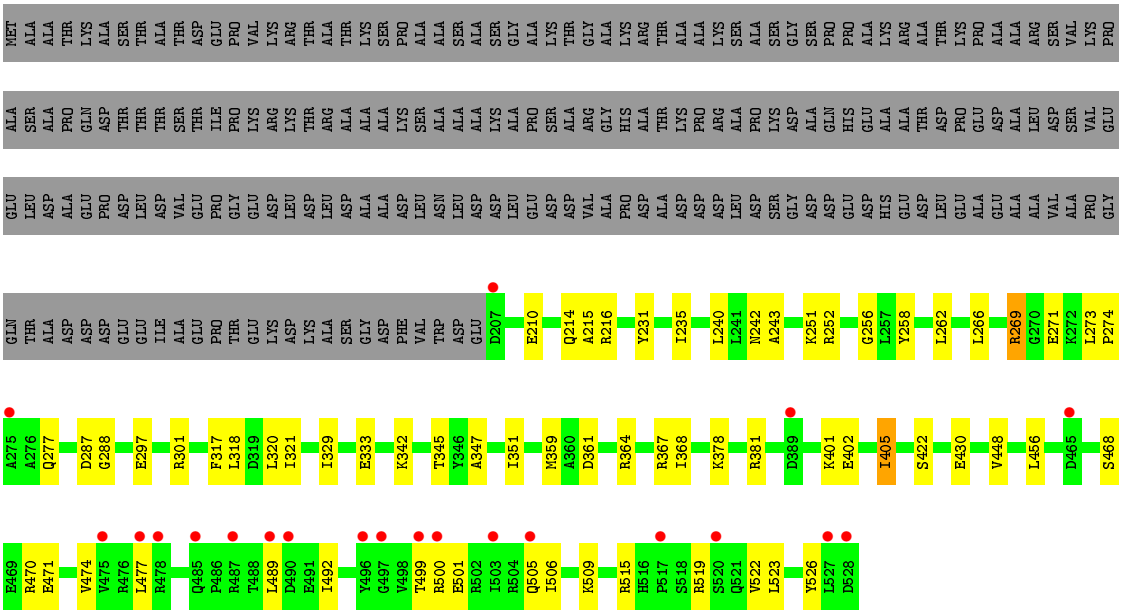




• Molecule 4: DNA-directed RNA polymerase subunit omega



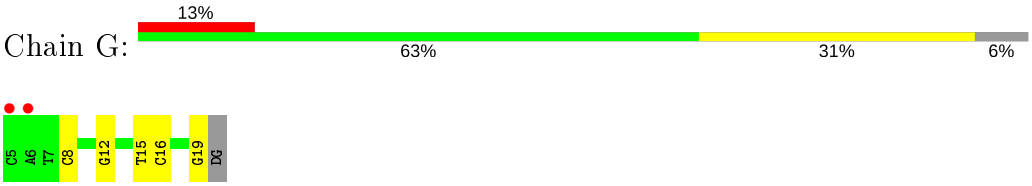
• Molecule 5: RNA polymerase sigma factor SigA



• Molecule 6: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*AP*GP*CP*TP*GP*TP*CP *AP*CP*GP*GP*AP*TP*G)-3')

• Molecule 7: DNA (5'-D(*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*CP*AP*GP*G)-3')

Chain G:



• Molecule 8: RNA (5'-R(*GP*GP*A)-3')

Chain I:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	150.05Å 167.39Å 195.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.81 – 3.80 49.16 – 3.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (48.81-3.80) 89.1 (49.16-3.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.79 (at 3.77Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.204 , 0.267 0.209 , 0.266	Depositor DCC
R_{free} test set	2000 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 12.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	26105	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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: ZN, RFP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.23	0/1730	0.44	0/2354
1	B	0.22	0/1730	0.45	0/2355
2	C	0.25	0/8873	0.43	1/12031 (0.0%)
3	D	0.25	0/10049	0.42	0/13587
4	E	0.27	0/650	0.44	0/886
5	F	0.25	0/2585	0.41	0/3485
6	H	0.58	1/535 (0.2%)	0.92	0/826
7	G	0.54	0/339	0.86	0/521
8	I	0.40	0/73	0.92	0/113
All	All	0.26	1/26564 (0.0%)	0.46	1/36158 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	13	DT	O3'-P	5.19	1.67	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	48	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1704	0	1741	26	0
1	B	1705	0	1730	28	0
2	C	8714	0	8636	138	0
3	D	9884	0	9941	157	0
4	E	637	0	635	15	0
5	F	2555	0	2579	43	0
6	H	476	0	261	11	0
7	G	303	0	170	4	0
8	I	65	0	35	6	0
9	C	59	0	58	10	0
10	D	2	0	0	0	0
11	D	1	0	0	0	0
All	All	26105	0	25786	382	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 7.

All (382) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:891:CYS:HB2	3:D:968:CYS:SG	1.95	1.06
3:D:913:ASP:OD1	3:D:914:PRO:HD2	1.60	1.01
3:D:913:ASP:OD1	3:D:914:PRO:CD	2.20	0.89
3:D:908:GLY:O	3:D:909:THR:OG1	1.92	0.88
6:H:16:DC:O2	7:G:12:DG:N2	2.08	0.86
3:D:891:CYS:SG	3:D:975:CYS:HB3	2.18	0.83
2:C:230:ARG:HH12	7:G:8:DC:H5"	1.43	0.82
2:C:454:ARG:HH22	9:C:1201:RFP:H19C	1.47	0.80
3:D:905:ALA:HB3	3:D:908:GLY:O	1.85	0.76
2:C:305:ARG:HH12	6:H:10:DA:H62	1.33	0.75
2:C:1122:LYS:HE2	2:C:1148:ARG:HG2	1.71	0.73
3:D:1090:LYS:HB3	3:D:1092:GLU:HG2	1.71	0.72
3:D:910:LEU:O	3:D:910:LEU:HD12	1.91	0.71
3:D:107:PHE:HZ	3:D:126:GLU:HG2	1.54	0.71
2:C:113:ASP:HB2	2:C:132:PRO:HG2	1.71	0.70
3:D:891:CYS:SG	3:D:970:THR:OG1	2.49	0.70
4:E:60:ARG:NE	4:E:98:GLU:OE2	2.22	0.70
2:C:101:GLY:O	2:C:142:ASN:ND2	2.25	0.69
2:C:189:GLU:HB2	2:C:367:THR:HG21	1.75	0.69
5:F:256:GLY:HA3	5:F:288:GLY:HA3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:401:LYS:HA	5:F:405:ILE:HA	1.76	0.68
3:D:473:LYS:HZ3	5:F:448:VAL:HG11	1.58	0.68
3:D:1164:ARG:NH2	3:D:1216:ALA:O	2.27	0.68
2:C:815:THR:HG22	2:C:817:GLU:H	1.59	0.68
3:D:913:ASP:OD1	3:D:914:PRO:N	2.27	0.67
3:D:130:TYR:OH	3:D:379:ASP:OD2	2.11	0.67
2:C:401:ARG:HA	2:C:404:MET:HE2	1.76	0.67
2:C:473:ARG:NH2	2:C:492:PRO:O	2.28	0.67
2:C:43:LYS:NZ	2:C:544:ALA:O	2.29	0.66
3:D:1165:VAL:HG12	3:D:1205:PRO:HA	1.76	0.66
3:D:638:THR:HG23	3:D:639:GLN:HG2	1.77	0.66
5:F:477:LEU:HD13	5:F:492:ILE:HG23	1.77	0.66
2:C:441:ASP:H	2:C:451:HIS:HD2	1.43	0.65
3:D:891:CYS:CB	3:D:968:CYS:SG	2.71	0.65
2:C:974:THR:HG23	2:C:980:ALA:H	1.63	0.64
3:D:136:ILE:HD11	3:D:235:ILE:HD11	1.79	0.64
1:A:213:LYS:HD3	1:B:227:VAL:HG23	1.79	0.64
5:F:522:VAL:HG23	5:F:523:LEU:HD12	1.79	0.63
2:C:1024:THR:H	3:D:730:THR:HG21	1.62	0.63
5:F:470:ARG:HH11	5:F:506:ILE:HD11	1.64	0.63
5:F:470:ARG:HB3	5:F:506:ILE:HD13	1.80	0.62
9:C:1201:RFP:H411	8:I:1:G:H5”	1.81	0.62
3:D:907:ASP:N	3:D:907:ASP:OD1	2.26	0.62
2:C:475:VAL:O	3:D:854:HIS:ND1	2.33	0.61
2:C:599:HIS:HB3	2:C:928:ILE:HD12	1.83	0.60
2:C:168:ILE:HG12	2:C:431:PHE:HB3	1.84	0.60
5:F:242:ASN:OD1	5:F:243:ALA:N	2.35	0.60
1:A:152:ASN:HB3	1:A:163:PRO:HB3	1.84	0.59
1:B:75:GLU:O	1:B:79:ASN:ND2	2.32	0.59
9:C:1201:RFP:HN1	9:C:1201:RFP:H18C	1.67	0.59
3:D:107:PHE:CZ	3:D:126:GLU:HG2	2.37	0.59
3:D:997:ILE:HD11	3:D:1248:LEU:HD13	1.84	0.59
2:C:348:LEU:HD13	2:C:365:VAL:HG12	1.83	0.59
2:C:104:SER:HB3	2:C:140:ILE:HB	1.84	0.58
3:D:102:THR:HG22	3:D:313:VAL:HG22	1.84	0.58
3:D:915:TYR:HA	3:D:1143:ARG:HH12	1.68	0.58
1:B:27:GLU:HG3	1:B:28:PRO:HD2	1.86	0.58
1:A:214:THR:HA	1:B:230:GLU:HG2	1.86	0.58
2:C:317:ASN:O	2:C:321:GLY:N	2.33	0.58
2:C:441:ASP:H	2:C:451:HIS:CD2	2.21	0.57
3:D:1051:GLY:HA2	3:D:1069:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:600:GLN:HB2	3:D:609:THR:HB	1.87	0.57
1:A:64:THR:OG1	1:A:65:THR:N	2.38	0.56
2:C:211:TRP:HB2	2:C:227:ASP:HA	1.85	0.56
3:D:902:ALA:HB1	3:D:911:ILE:O	2.04	0.56
3:D:930:VAL:HG22	3:D:936:VAL:HG12	1.85	0.56
2:C:1148:ARG:NH1	3:D:86:LYS:HG3	2.20	0.56
3:D:1089:PHE:HA	3:D:1095:SER:HA	1.87	0.56
5:F:252:ARG:NH1	5:F:287:ASP:OD1	2.33	0.56
2:C:1045:SER:OG	2:C:1046:THR:N	2.36	0.56
9:C:1201:RFP:O12	9:C:1201:RFP:O4	2.23	0.56
3:D:1090:LYS:HG2	3:D:1091:HIS:H	1.69	0.56
2:C:185:VAL:HG12	2:C:316:VAL:HG22	1.88	0.56
2:C:239:LYS:NZ	2:C:265:ASP:OD2	2.37	0.56
3:D:901:LEU:O	3:D:901:LEU:HD13	2.06	0.56
5:F:240:LEU:HD21	5:F:301:ARG:HD2	1.87	0.55
3:D:45:GLY:H	3:D:48:CYS:HB2	1.71	0.55
2:C:279:ARG:HD3	5:F:215:ALA:HB1	1.87	0.55
6:H:15:DT:H2"	6:H:16:DC:H5'	1.88	0.55
3:D:104:ILE:HD12	3:D:379:ASP:HB3	1.87	0.55
3:D:899:VAL:HG11	3:D:920:ALA:HB2	1.87	0.55
9:C:1201:RFP:H382	8:I:2:G:N7	2.22	0.55
5:F:506:ILE:HA	5:F:509:LYS:HD2	1.87	0.55
3:D:565:ILE:HG23	3:D:575:ALA:HB3	1.89	0.54
3:D:1038:ARG:NH1	6:H:18:DC:O3'	2.41	0.54
3:D:1055:LEU:HB2	3:D:1101:ASP:HB3	1.90	0.54
3:D:266:GLU:HA	3:D:310:MET:HE1	1.89	0.54
3:D:373:MET:SD	5:F:318:LEU:HB3	2.48	0.54
3:D:913:ASP:HB3	3:D:916:ILE:HG13	1.89	0.54
1:A:56:ILE:HG12	1:A:136:VAL:HG13	1.90	0.54
3:D:46:LEU:O	3:D:325:ARG:NH2	2.27	0.54
2:C:513:GLU:HB3	2:C:530:TYR:HB3	1.89	0.53
5:F:505:GLN:HG3	5:F:509:LYS:HE3	1.90	0.53
5:F:320:LEU:HD21	5:F:359:MET:HE3	1.91	0.53
1:B:72:ASP:OD1	1:B:73:VAL:N	2.41	0.52
3:D:113:ARG:H	3:D:113:ARG:HD2	1.74	0.52
3:D:365:ILE:HG21	5:F:297:GLU:HG2	1.91	0.52
5:F:474:VAL:HA	5:F:477:LEU:HD12	1.90	0.52
2:C:377:ARG:NH2	2:C:383:GLU:OE1	2.42	0.52
2:C:549:ASP:HB3	2:C:553:ARG:H	1.74	0.52
7:G:15:DT:H2'	7:G:16:DC:C6	2.45	0.52
9:C:1201:RFP:N2	9:C:1201:RFP:O12	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1201:RFP:H381	8:I:1:G:H8	1.75	0.52
3:D:1244:LYS:O	3:D:1246:ASN:N	2.43	0.51
3:D:567:SER:HB2	3:D:574:LEU:HG	1.92	0.51
3:D:908:GLY:C	3:D:909:THR:HG1	2.00	0.51
3:D:1085:ARG:HA	3:D:1112:MET:HA	1.92	0.51
1:B:90:ASP:HA	1:B:142:ARG:HD3	1.92	0.51
3:D:1069:ASP:OD2	3:D:1104:HIS:NE2	2.43	0.51
2:C:1020:PRO:HB2	2:C:1021:TYR:CD2	2.46	0.51
2:C:211:TRP:HH2	6:H:14:DG:OP1	1.92	0.51
1:A:129:ASN:ND2	2:C:652:GLU:HG3	2.25	0.51
5:F:468:SER:HB3	5:F:471:GLU:HG3	1.93	0.51
1:B:170:PRO:HA	1:B:199:LYS:HD2	1.91	0.51
3:D:589:THR:HG21	3:D:688:MET:HG2	1.93	0.51
3:D:965:VAL:HG13	3:D:974:VAL:HG11	1.93	0.51
3:D:341:ASN:O	3:D:345:ARG:HB2	2.11	0.51
3:D:676:LEU:HD23	3:D:716:LEU:HD23	1.93	0.51
2:C:1148:ARG:NH1	3:D:86:LYS:O	2.44	0.51
2:C:287:PRO:HD2	5:F:216:ARG:HA	1.91	0.51
2:C:344:TYR:OH	2:C:365:VAL:HA	2.11	0.50
3:D:1139:GLN:O	3:D:1143:ARG:HG2	2.10	0.50
2:C:762:THR:HG23	2:C:764:LEU:H	1.76	0.50
2:C:737:LEU:HB2	2:C:898:ILE:HG12	1.93	0.50
1:B:55:ARG:HB2	1:B:137:GLU:HB3	1.94	0.50
3:D:320:ILE:HG22	3:D:344:TYR:HE2	1.75	0.50
2:C:756:GLU:OE2	2:C:870:ARG:NE	2.40	0.49
3:D:139:VAL:HG12	3:D:231:PRO:HD3	1.94	0.49
2:C:614:GLN:NE2	8:I:2:G:OP1	2.45	0.49
1:A:89:GLU:HG3	1:A:93:VAL:HG11	1.94	0.49
6:H:11:DG:H5"	6:H:12:DC:C4	2.48	0.49
5:F:347:ALA:O	5:F:351:ILE:HG13	2.11	0.49
3:D:442:GLY:HA3	3:D:523:GLN:HB2	1.95	0.49
4:E:38:PRO:HD2	4:E:96:LEU:HD23	1.95	0.49
2:C:959:LEU:HD12	2:C:960:PRO:HD2	1.95	0.49
3:D:36:TYR:CZ	3:D:37:ARG:HG3	2.47	0.49
5:F:499:THR:HG23	5:F:500:ARG:HD2	1.95	0.49
1:B:45:SER:OG	1:B:214:THR:HG21	2.13	0.49
2:C:38:ARG:HA	2:C:971:ILE:HG13	1.93	0.49
2:C:597:LEU:HD23	2:C:976:VAL:HG11	1.95	0.49
2:C:536:GLU:OE2	2:C:562:ARG:NH1	2.40	0.48
3:D:588:LEU:HD12	3:D:589:THR:HG23	1.95	0.48
2:C:485:PRO:O	3:D:857:ARG:NH2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1125:LEU:HD22	2:C:1135:VAL:HG11	1.94	0.48
3:D:339:ASP:OD1	5:F:422:SER:OG	2.25	0.48
1:A:37:SER:O	1:A:41:THR:OG1	2.29	0.48
5:F:499:THR:OG1	5:F:500:ARG:N	2.42	0.48
2:C:1052:ILE:O	3:D:89:ARG:NH1	2.45	0.48
2:C:102:SER:O	2:C:141:ASN:ND2	2.47	0.48
3:D:1092:GLU:HG3	3:D:1094:GLY:H	1.78	0.48
3:D:670:ARG:O	3:D:674:ASN:ND2	2.36	0.48
2:C:597:LEU:HB3	2:C:976:VAL:HG13	1.95	0.48
3:D:67:ARG:HB3	3:D:69:ARG:HG2	1.94	0.48
4:E:56:TYR:HE2	4:E:99:ILE:HG12	1.78	0.48
1:B:44:SER:O	1:B:144:ARG:HB3	2.14	0.48
3:D:1110:GLN:NE2	3:D:1112:MET:O	2.43	0.48
6:H:15:DT:H2"	6:H:16:DC:H6	1.78	0.48
2:C:464:SER:HB3	2:C:467:ARG:HG3	1.96	0.48
2:C:653:VAL:HG12	2:C:692:ALA:HB2	1.96	0.48
5:F:378:LYS:HD3	5:F:381:ARG:HH11	1.78	0.48
3:D:437:LYS:HE2	4:E:33:LEU:HD11	1.96	0.48
5:F:262:LEU:O	5:F:266:LEU:HG	2.14	0.48
3:D:740:PRO:HD3	3:D:792:HIS:ND1	2.29	0.47
2:C:314:TYR:CZ	2:C:318:LYS:HD3	2.49	0.47
2:C:642:VAL:HB	2:C:703:ALA:HB3	1.96	0.47
2:C:720:LEU:HD23	2:C:913:VAL:HA	1.95	0.47
4:E:33:LEU:H	4:E:33:LEU:HD23	1.79	0.47
2:C:211:TRP:NE1	6:H:13:DT:O2	2.45	0.47
2:C:486:ILE:HD11	3:D:849:TYR:HE2	1.78	0.47
5:F:342:LYS:O	5:F:345:THR:HG22	2.14	0.47
2:C:809:LYS:HD2	2:C:833:ARG:HD3	1.95	0.47
2:C:1112:ILE:HG13	3:D:548:SER:HA	1.95	0.47
1:A:100:GLN:HG2	1:A:101:GLY:H	1.80	0.47
2:C:115:VAL:HG11	2:C:129:TYR:CE1	2.49	0.47
2:C:1055:GLN:NE2	3:D:420:LYS:HG2	2.29	0.47
3:D:274:ALA:HB1	3:D:278:ARG:HH12	1.79	0.47
3:D:67:ARG:HD2	3:D:69:ARG:NE	2.29	0.47
1:B:27:GLU:HB3	1:B:30:PHE:HD2	1.79	0.47
2:C:233:PRO:HB2	2:C:236:VAL:HG23	1.97	0.47
5:F:273:LEU:HD13	5:F:277:GLN:HB3	1.95	0.47
3:D:101:VAL:HG23	3:D:375:GLN:CD	2.35	0.47
5:F:489:LEU:HD23	5:F:489:LEU:H	1.79	0.47
5:F:515:ARG:O	5:F:519:ARG:N	2.46	0.47
5:F:456:LEU:HD12	5:F:526:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1044:ARG:HH12	2:C:1048:PRO:HD2	1.80	0.46
3:D:473:LYS:HD2	5:F:448:VAL:HG21	1.97	0.46
2:C:313:ARG:NH1	2:C:332:THR:O	2.49	0.46
3:D:369:ASN:O	3:D:373:MET:HG3	2.15	0.46
3:D:595:ASP:HB3	3:D:631:ALA:HB2	1.96	0.46
3:D:69:ARG:HD2	3:D:70:PHE:CZ	2.51	0.46
2:C:587:VAL:HB	2:C:591:THR:HB	1.97	0.46
2:C:596:PHE:HB3	2:C:599:HIS:HD2	1.80	0.46
4:E:96:LEU:HA	4:E:99:ILE:HD12	1.96	0.46
2:C:818:GLU:OE2	2:C:822:ARG:NH1	2.48	0.46
3:D:891:CYS:O	3:D:892:GLN:HB2	2.15	0.46
5:F:269:ARG:NH1	5:F:271:GLU:OE1	2.47	0.46
3:D:114:LEU:HB3	3:D:125:LEU:HD21	1.96	0.46
3:D:530:GLU:HB2	3:D:578:ARG:HD2	1.96	0.46
2:C:1136:GLU:OE1	3:D:11:ARG:NH1	2.49	0.46
3:D:137:THR:OG1	3:D:253:THR:O	2.32	0.46
3:D:503:THR:HG23	3:D:508:GLY:HA3	1.98	0.46
1:A:225:LEU:HD13	1:A:225:LEU:H	1.81	0.46
1:B:92:PRO:HB3	1:B:141:GLU:HG2	1.97	0.46
2:C:1045:SER:HB3	3:D:450:GLU:O	2.16	0.46
6:H:18:DC:H2"	6:H:19:DG:C8	2.49	0.46
2:C:46:GLU:N	2:C:47:PRO:HD3	2.31	0.46
5:F:231:TYR:CE2	5:F:235:ILE:HD11	2.51	0.46
3:D:114:LEU:HD23	3:D:114:LEU:HA	1.80	0.46
9:C:1201:RFP:C18	9:C:1201:RFP:HN1	2.28	0.45
2:C:598:GLU:HA	3:D:849:TYR:CE1	2.51	0.45
2:C:600:ASP:OD2	2:C:889:HIS:ND1	2.32	0.45
3:D:308:SER:HA	3:D:309:PRO:HD3	1.74	0.45
5:F:430:GLU:HB2	7:G:19:DG:N2	2.31	0.45
1:B:148:PRO:O	1:B:152:ASN:ND2	2.50	0.45
2:C:1084:THR:N	3:D:554:GLU:OE2	2.39	0.45
5:F:318:LEU:HA	5:F:321:ILE:HD12	1.98	0.45
3:D:365:ILE:HG23	3:D:366:ILE:HG13	1.98	0.45
3:D:409:LYS:O	3:D:415:GLN:HB2	2.16	0.45
3:D:707:ILE:HD11	4:E:32:PRO:HB3	1.98	0.45
1:A:175:THR:OG1	1:A:176:TYR:N	2.49	0.45
2:C:894:VAL:HG22	3:D:536:PHE:O	2.17	0.45
6:H:22:DT:H1'	6:H:23:DG:H5'	1.99	0.45
2:C:183:PRO:HB2	2:C:312:GLY:HA2	1.99	0.45
3:D:153:ALA:O	3:D:157:VAL:HG23	2.17	0.45
2:C:1044:ARG:NH1	2:C:1063:PHE:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:1201:RFP:H381	8:I:1:G:C8	2.52	0.45
3:D:760:PHE:CG	3:D:770:ARG:HD2	2.52	0.45
3:D:873:LEU:HA	3:D:876:ARG:HE	1.81	0.45
1:B:99:LYS:HD3	1:B:105:VAL:HG22	1.99	0.45
2:C:773:ILE:HD11	2:C:804:GLY:HA2	1.98	0.45
3:D:457:MET:HE3	3:D:457:MET:HB2	1.83	0.45
1:B:171:VAL:HG22	1:B:198:THR:HG22	1.99	0.45
2:C:257:ILE:HD11	2:C:346:VAL:HG23	1.99	0.45
2:C:927:ASN:O	2:C:930:GLN:HG2	2.17	0.45
3:D:921:TYR:OH	3:D:946:ASP:OD1	2.25	0.45
1:B:178:VAL:HG22	1:B:192:LEU:HD13	1.97	0.44
2:C:758:ASP:N	2:C:758:ASP:OD1	2.50	0.44
3:D:321:PRO:HA	3:D:322:PRO:HD3	1.83	0.44
3:D:505:HIS:CE1	3:D:507:LEU:HB2	2.52	0.44
4:E:46:ARG:NE	4:E:102:ASP:OD1	2.40	0.44
1:A:197:GLU:OE1	2:C:996:ARG:NH1	2.38	0.44
2:C:1119:GLU:O	2:C:1123:VAL:HG23	2.18	0.44
2:C:111:ARG:NH2	2:C:151:THR:OG1	2.51	0.44
2:C:408:ASP:N	2:C:408:ASP:OD1	2.45	0.44
3:D:676:LEU:HG	3:D:715:LYS:HB3	2.00	0.44
1:A:130:ASP:O	1:A:131:LYS:HG2	2.18	0.44
3:D:581:MET:HG3	3:D:721:PHE:CE1	2.51	0.44
2:C:1141:ASP:OD1	2:C:1142:GLY:N	2.50	0.44
2:C:232:GLN:OE1	2:C:280:LYS:HG3	2.17	0.44
2:C:438:GLN:HE22	9:C:1201:RFP:C8	2.30	0.44
2:C:885:LEU:HD12	2:C:895:ILE:HD11	2.00	0.44
4:E:84:GLU:H	4:E:84:GLU:CD	2.20	0.44
2:C:733:ASP:OD2	2:C:925:ARG:NH2	2.51	0.44
2:C:378:LEU:HD21	2:C:455:LEU:HD22	1.98	0.44
5:F:477:LEU:HB3	5:F:492:ILE:HD13	2.00	0.44
1:A:150:VAL:HA	1:A:153:ARG:HH12	1.83	0.44
2:C:708:THR:HA	2:C:712:GLU:O	2.18	0.44
3:D:1010:LEU:HD12	3:D:1028:LEU:HB2	1.99	0.44
4:E:95:ALA:O	4:E:99:ILE:HG13	2.18	0.44
3:D:1031:VAL:HG22	3:D:1141:VAL:HG11	2.00	0.44
3:D:1087:ARG:HG2	3:D:1098:VAL:HG22	2.00	0.44
1:A:223:ARG:HD3	1:B:213:LYS:HB2	2.00	0.43
1:A:62:GLU:HG3	1:A:77:ILE:HD12	2.00	0.43
3:D:772:GLU:O	3:D:776:GLU:HG2	2.18	0.43
4:E:40:ILE:O	4:E:44:LEU:HG	2.18	0.43
1:A:14:LEU:HD23	1:A:19:SER:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:400:LYS:HA	3:D:400:LYS:HD3	1.87	0.43
3:D:781:ALA:O	3:D:785:VAL:HG23	2.18	0.43
5:F:364:ARG:HG3	5:F:368:ILE:HG12	2.00	0.43
2:C:281:LEU:HD22	2:C:282:ARG:HG3	1.99	0.43
2:C:756:GLU:HG3	2:C:870:ARG:HG2	1.99	0.43
3:D:1247:GLY:O	3:D:1251:ASN:ND2	2.43	0.43
3:D:403:SER:O	3:D:407:LYS:HG3	2.18	0.43
2:C:220:ASP:HB3	2:C:257:ILE:HG22	1.99	0.43
2:C:817:GLU:N	2:C:817:GLU:OE1	2.52	0.43
3:D:460:LEU:HA	3:D:460:LEU:HD23	1.92	0.43
3:D:293:LEU:HD21	3:D:1177:PRO:HG2	2.01	0.43
5:F:274:PRO:HG2	5:F:277:GLN:HB2	2.01	0.43
1:A:87:SER:O	1:A:142:ARG:NH1	2.44	0.43
1:B:77:ILE:HG22	1:B:81:LYS:HE3	2.01	0.43
2:C:157:PHE:HA	2:C:158:PRO:HD3	1.93	0.43
2:C:465:ARG:HD3	2:C:492:PRO:HB2	2.00	0.43
3:D:1152:LYS:O	3:D:1156:VAL:HG23	2.18	0.43
3:D:925:LEU:HD12	3:D:962:VAL:HG12	2.01	0.43
2:C:484:CYS:HB2	2:C:588:SER:HB3	2.01	0.42
3:D:123:LYS:HD2	3:D:123:LYS:HA	1.76	0.42
3:D:230:ALA:N	3:D:233:GLN:OE1	2.51	0.42
5:F:329:ILE:O	5:F:333:GLU:HG2	2.19	0.42
2:C:1044:ARG:NH1	2:C:1048:PRO:HD2	2.34	0.42
2:C:1091:ILE:HB	2:C:1102:VAL:HG21	2.00	0.42
3:D:384:ASN:HB2	3:D:401:SER:HB3	2.01	0.42
3:D:428:SER:HB3	3:D:522:ILE:HG13	1.99	0.42
2:C:546:SER:HA	2:C:547:PRO:HD3	1.88	0.42
3:D:1176:LEU:HD12	3:D:1176:LEU:H	1.84	0.42
3:D:789:LEU:HD22	3:D:793:TYR:CE2	2.53	0.42
5:F:345:THR:HB	6:H:4:DA:H8	1.84	0.42
2:C:601:ASP:OD2	2:C:602:ALA:N	2.52	0.42
2:C:928:ILE:H	2:C:928:ILE:HG13	1.44	0.42
1:A:120:ASN:N	1:A:120:ASN:OD1	2.51	0.42
2:C:150:GLN:HG2	2:C:414:PRO:HG2	2.01	0.42
3:D:177:LEU:HD13	3:D:201:GLY:HA3	2.01	0.42
2:C:251:ARG:NH2	2:C:343:GLU:OE1	2.46	0.42
2:C:173:ARG:NH1	2:C:437:SER:O	2.53	0.42
3:D:666:THR:HG21	3:D:683:PHE:CE2	2.53	0.42
1:A:136:VAL:HG12	1:A:137:GLU:H	1.85	0.42
1:A:40:ARG:HD2	2:C:1013:GLY:O	2.20	0.42
3:D:1156:VAL:O	3:D:1160:GLN:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1111:ASN:OD1	4:E:65:ASN:ND2	2.53	0.42
1:B:45:SER:OG	1:B:45:SER:O	2.37	0.42
2:C:48:LEU:HD12	2:C:528:ILE:HD13	2.02	0.42
2:C:544:ALA:HB2	2:C:580:ASP:HB2	2.02	0.42
3:D:732:SER:OG	3:D:733:MET:N	2.53	0.42
3:D:945:GLY:O	3:D:949:ILE:HG12	2.20	0.42
1:B:146:TYR:O	3:D:624:ARG:NE	2.53	0.42
1:B:208:LEU:O	1:B:212:GLY:N	2.52	0.42
3:D:1068:PRO:HB2	3:D:1071:GLY:O	2.20	0.42
1:B:84:VAL:HG23	1:B:119:HIS:HB2	2.01	0.41
2:C:1114:GLU:HA	2:C:1115:PRO:HD3	1.88	0.41
4:E:90:LYS:HA	4:E:90:LYS:HD3	1.86	0.41
2:C:476:HIS:CG	2:C:477:PRO:HD2	2.55	0.41
2:C:958:ARG:HD2	2:C:958:ARG:N	2.36	0.41
3:D:539:ASP:OD1	8:I:3:A:O3'	2.31	0.41
3:D:717:LYS:HE2	3:D:717:LYS:HB3	1.88	0.41
1:B:39:ARG:HH21	1:B:173:LYS:NZ	2.18	0.41
2:C:1041:ILE:HD11	3:D:447:MET:HG3	2.02	0.41
2:C:212:LEU:HB2	2:C:300:PHE:HE1	1.86	0.41
2:C:503:TYR:HB3	2:C:515:PRO:HG3	2.01	0.41
2:C:735:ILE:HD12	2:C:885:LEU:HB2	2.02	0.41
2:C:96:ILE:HD13	2:C:397:GLU:HG3	2.01	0.41
3:D:1127:PRO:O	3:D:1130:VAL:HG12	2.20	0.41
1:B:84:VAL:HG12	1:B:199:LYS:HD3	2.01	0.41
3:D:1065:THR:HG23	3:D:1076:VAL:HB	2.02	0.41
3:D:453:LYS:O	3:D:457:MET:HG3	2.20	0.41
3:D:990:ASP:OD2	4:E:49:SER:HB2	2.20	0.41
2:C:690:VAL:HG11	2:C:696:VAL:HG11	2.02	0.41
2:C:933:GLU:O	2:C:937:GLY:N	2.53	0.41
3:D:218:ARG:O	3:D:222:ILE:HG13	2.20	0.41
3:D:264:LEU:HA	3:D:264:LEU:HD13	1.94	0.41
1:B:173:LYS:HE2	3:D:619:ILE:HD13	2.01	0.41
2:C:400:VAL:O	2:C:404:MET:HG3	2.20	0.41
1:A:217:GLU:HG2	1:B:232:ILE:HG13	2.02	0.41
2:C:1084:THR:O	2:C:1088:LEU:HG	2.21	0.41
2:C:115:VAL:HG22	2:C:131:ALA:HB2	2.01	0.41
2:C:596:PHE:HB3	2:C:599:HIS:CD2	2.54	0.41
1:A:18:ARG:NH1	2:C:997:ASP:OD1	2.47	0.41
3:D:89:ARG:HG2	3:D:323:GLU:HB2	2.03	0.41
3:D:773:ALA:O	3:D:777:ILE:HG13	2.20	0.41
2:C:720:LEU:HD13	2:C:1027:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1067:ARG:NH2	3:D:415:GLN:O	2.47	0.41
3:D:737:LEU:O	3:D:818:ALA:HB1	2.21	0.41
3:D:770:ARG:NH1	3:D:771:ASN:OD1	2.53	0.41
2:C:239:LYS:HZ3	2:C:268:VAL:HG23	1.85	0.41
2:C:200:HIS:CD2	2:C:348:LEU:HG	2.56	0.41
2:C:763:LYS:HD3	2:C:763:LYS:HA	1.92	0.41
3:D:827:PRO:HG3	3:D:854:HIS:NE2	2.35	0.41
3:D:797:ASN:HA	3:D:798:PRO:HD3	1.79	0.41
3:D:903:GLU:O	3:D:911:ILE:HB	2.20	0.41
1:A:149:ALA:HB2	1:A:165:ASP:N	2.36	0.41
2:C:377:ARG:HH22	2:C:383:GLU:CD	2.25	0.41
2:C:568:VAL:HG21	3:D:847:LEU:HD23	2.02	0.41
3:D:1187:GLU:O	3:D:1191:ARG:HB2	2.21	0.41
3:D:525:HIS:HA	3:D:526:PRO:HD3	1.82	0.41
4:E:38:PRO:HA	4:E:39:PRO:HD3	1.98	0.41
5:F:210:GLU:O	5:F:214:GLN:HG2	2.21	0.41
1:B:110:ILE:O	1:B:112:PRO:HD3	2.20	0.40
2:C:519:VAL:HG22	2:C:524:VAL:HA	2.04	0.40
3:D:925:LEU:HD11	3:D:960:VAL:HG11	2.04	0.40
2:C:182:SER:HB2	2:C:377:ARG:HB2	2.04	0.40
3:D:1254:ILE:HD11	3:D:1256:LYS:HB2	2.04	0.40
3:D:20:ILE:HD12	3:D:318:PRO:HD3	2.03	0.40
2:C:731:TYR:HE1	3:D:579:LEU:HB2	1.86	0.40
5:F:317:PHE:O	5:F:321:ILE:HG13	2.21	0.40
1:A:77:ILE:HG22	1:A:81:LYS:HE2	2.03	0.40
1:B:212:GLY:O	1:B:216:VAL:HG23	2.22	0.40
2:C:389:ILE:O	2:C:393:MET:HG2	2.21	0.40
2:C:420:ILE:O	2:C:424:VAL:HG23	2.21	0.40
2:C:723:ILE:O	3:D:730:THR:HG23	2.21	0.40
5:F:515:ARG:O	5:F:519:ARG:HG2	2.22	0.40
3:D:402:LEU:HD23	3:D:402:LEU:HA	1.96	0.40
3:D:832:ILE:HG22	3:D:834:ARG:H	1.86	0.40
1:A:83:LEU:HG	1:A:85:VAL:HG23	2.04	0.40
2:C:641:VAL:HG11	2:C:708:THR:HG21	2.04	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	222/347 (64%)	211 (95%)	10 (4%)	1 (0%)	29	66
1	B	221/347 (64%)	202 (91%)	17 (8%)	2 (1%)	17	54
2	C	1124/1178 (95%)	1052 (94%)	66 (6%)	6 (0%)	29	66
3	D	1261/1316 (96%)	1188 (94%)	68 (5%)	5 (0%)	34	70
4	E	79/110 (72%)	77 (98%)	1 (1%)	1 (1%)	12	48
5	F	320/528 (61%)	303 (95%)	15 (5%)	2 (1%)	25	62
All	All	3227/3826 (84%)	3033 (94%)	177 (6%)	17 (0%)	29	66

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	678	PRO
2	C	47	PRO
3	D	1245	LEU
1	A	184	GLU
5	F	405	ILE
2	C	441	ASP
2	C	1148	ARG
3	D	593	PRO
5	F	501	GLU
1	B	226	ASN
3	D	607	PRO
3	D	658	PRO
2	C	32	VAL
1	B	227	VAL
2	C	33	PRO
2	C	520	VAL
4	E	75	ILE

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	
1	A	192/297 (65%)	189 (98%)	3 (2%)	62	79
1	B	191/297 (64%)	190 (100%)	1 (0%)	88	94
2	C	948/998 (95%)	933 (98%)	15 (2%)	62	79
3	D	1047/1095 (96%)	1024 (98%)	23 (2%)	52	72
4	E	68/90 (76%)	66 (97%)	2 (3%)	42	67
5	F	271/427 (64%)	265 (98%)	6 (2%)	52	72
All	All	2717/3204 (85%)	2667 (98%)	50 (2%)	59	77

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ILE
1	A	182	ARG
1	A	225	LEU
1	B	17	ASN
2	C	48	LEU
2	C	180	VAL
2	C	185	VAL
2	C	373	PHE
2	C	439	PHE
2	C	447	SER
2	C	471	GLU
2	C	479	HIS
2	C	500	LEU
2	C	928	ILE
2	C	961	ASP
2	C	1044	ARG
2	C	1099	ARG
2	C	1120	SER
2	C	1148	ARG
3	D	7	PHE
3	D	14	LEU
3	D	62	CYS

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Mol	Chain	Res	Type
3	D	78	CYS
3	D	82	VAL
3	D	83	THR
3	D	114	LEU
3	D	535	ASP
3	D	582	VAL
3	D	583	THR
3	D	653	HIS
3	D	684	VAL
3	D	714	ASP
3	D	862	ASP
3	D	901	LEU
3	D	907	ASP
3	D	910	LEU
3	D	921	TYR
3	D	968	CYS
3	D	975	CYS
3	D	978	CYS
3	D	1009	GLN
3	D	1194	VAL
4	E	69	ASN
4	E	75	ILE
5	F	251	LYS
5	F	258	TYR
5	F	269	ARG
5	F	361	ASP
5	F	367	ARG
5	F	402	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	451	HIS
2	C	930	GLN
3	D	1139	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/3 (66%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	3	A

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
9	RFP	C	1201	-	63,63,63	2.62	11 (17%)	94,94,94	2.34	23 (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
9	RFP	C	1201	-	-	16/60/85/85	0/5/5/5

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	RFP	O4-C11	11.45	1.40	1.21
9	C	1201	RFP	C43-N2	8.16	1.50	1.27
9	C	1201	RFP	C17-C16	7.23	1.55	1.34
9	C	1201	RFP	C3-C43	5.29	1.56	1.46
9	C	1201	RFP	C15-N1	5.19	1.46	1.35
9	C	1201	RFP	O7-C25	-4.86	1.37	1.44
9	C	1201	RFP	C12-C11	-3.55	1.40	1.54
9	C	1201	RFP	C18-C17	3.45	1.54	1.43
9	C	1201	RFP	C6-C7	3.15	1.45	1.39
9	C	1201	RFP	O9-C23	-2.18	1.37	1.43
9	C	1201	RFP	C29-C28	2.03	1.41	1.30

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	RFP	C38-N4-C42	8.97	124.08	110.66
9	C	1201	RFP	C30-C16-C17	-7.45	105.39	123.42
9	C	1201	RFP	C3-C43-N2	-7.44	110.71	121.54
9	C	1201	RFP	O3-C6-C7	5.52	130.64	121.14
9	C	1201	RFP	C43-N2-N3	-4.80	113.70	120.43
9	C	1201	RFP	O7-C35-C36	4.61	119.57	111.09
9	C	1201	RFP	O4-C11-C5	-4.50	123.22	131.81
9	C	1201	RFP	C39-C40-N3	4.09	117.15	110.51
9	C	1201	RFP	C23-C24-C25	4.05	118.52	110.61
9	C	1201	RFP	C25-O7-C35	3.89	123.73	117.72
9	C	1201	RFP	C5-C10-C4	-3.79	120.05	124.03
9	C	1201	RFP	C2-C3-C43	-3.60	120.51	124.17
9	C	1201	RFP	C12-O5-C29	3.34	126.09	117.84
9	C	1201	RFP	C37-O6-C27	3.22	120.73	113.01
9	C	1201	RFP	C42-C41-N3	3.17	115.66	110.51
9	C	1201	RFP	C38-N4-C39	3.09	115.28	110.66
9	C	1201	RFP	O5-C12-C13	2.98	114.78	106.99
9	C	1201	RFP	C4-C3-C43	2.82	119.89	116.52
9	C	1201	RFP	C33-C24-C25	-2.58	106.78	111.40
9	C	1201	RFP	C25-C26-C27	2.46	118.75	112.02
9	C	1201	RFP	C5-C6-C7	-2.41	119.40	125.29
9	C	1201	RFP	C34-C26-C25	-2.22	107.41	111.40
9	C	1201	RFP	C26-C25-C24	-2.00	110.59	114.68

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	C	1201	RFP	C15-C16-C17-C18
9	C	1201	RFP	C26-C27-C28-C29
9	C	1201	RFP	O6-C27-C28-C29
9	C	1201	RFP	C26-C27-O6-C37
9	C	1201	RFP	C43-N2-N3-C40
9	C	1201	RFP	C43-N2-N3-C41
9	C	1201	RFP	C16-C17-C18-C19
9	C	1201	RFP	C36-C35-O7-C25
9	C	1201	RFP	C28-C27-O6-C37
9	C	1201	RFP	C3-C2-N1-C15
9	C	1201	RFP	C18-C19-C20-C31
9	C	1201	RFP	C30-C16-C17-C18
9	C	1201	RFP	C11-C12-O5-C29
9	C	1201	RFP	O3-C12-O5-C29
9	C	1201	RFP	C18-C19-C20-C21
9	C	1201	RFP	C17-C18-C19-C20

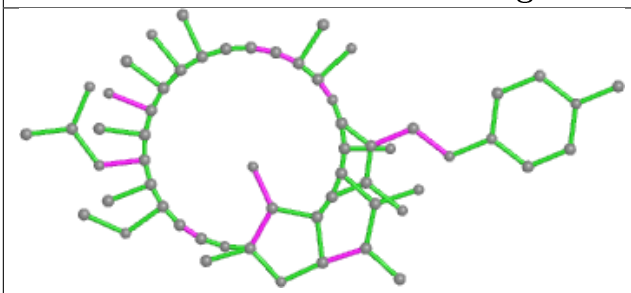
There are no ring outliers.

1 monomer is involved in 10 short contacts:

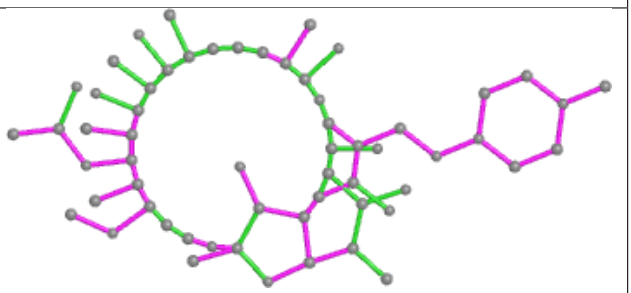
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	1201	RFP	10	0

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 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.

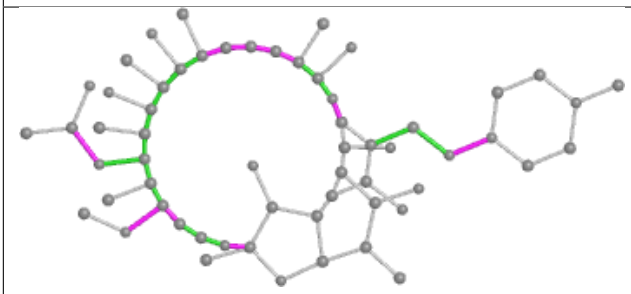
Ligand RFP C 1201



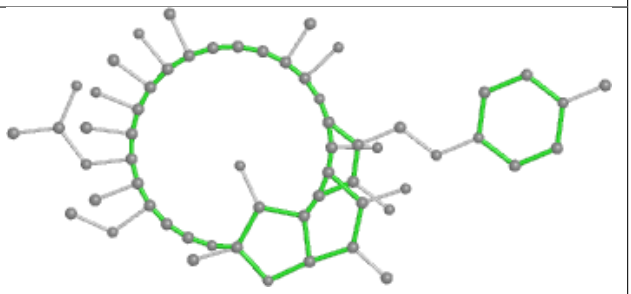
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	224/347 (64%)	-0.09	4 (1%) 68 61	15, 52, 119, 147	0
1	B	225/347 (64%)	0.72	27 (12%) 4 4	44, 89, 136, 161	0
2	C	1126/1178 (95%)	-0.21	34 (3%) 50 40	5, 33, 118, 143	0
3	D	1265/1316 (96%)	-0.28	19 (1%) 73 66	5, 36, 104, 148	0
4	E	81/110 (73%)	-0.21	1 (1%) 79 72	21, 43, 81, 96	0
5	F	322/528 (60%)	0.17	21 (6%) 18 14	10, 58, 163, 188	0
6	H	23/23 (100%)	0.13	0 100 100	28, 94, 161, 187	0
7	G	15/16 (93%)	0.35	2 (13%) 3 3	33, 67, 183, 186	0
8	I	3/3 (100%)	0.64	0 100 100	36, 36, 53, 68	0
All	All	3284/3868 (84%)	-0.12	108 (3%) 46 38	5, 43, 122, 188	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	500	ARG	5.1
5	F	499	THR	4.1
1	B	86	SER	4.1
2	C	235	THR	4.0
1	B	62	GLU	4.0
3	D	904	ARG	3.9
2	C	252	PHE	3.9
5	F	487	ARG	3.7
1	B	159	ILE	3.7
5	F	207	ASP	3.6
2	C	217	ASP	3.6
2	C	811	GLU	3.6
7	G	6	DA	3.4
3	D	187	GLU	3.3
2	C	221	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	223	ARG	3.1
1	B	87	SER	3.1
1	B	135	GLU	3.1
1	B	64	THR	3.0
1	B	63	PHE	3.0
5	F	528	ASP	3.0
3	D	909	THR	3.0
5	F	497	GLY	2.9
2	C	222	VAL	2.9
7	G	5	DC	2.9
5	F	478	ARG	2.9
3	D	186	ALA	2.8
2	C	220	ASP	2.8
3	D	906	PRO	2.8
2	C	219	ARG	2.7
1	B	228	GLU	2.7
1	B	229	ALA	2.7
2	C	192	ASP	2.6
5	F	490	ASP	2.6
5	F	489	LEU	2.6
2	C	775	ASN	2.6
2	C	218	LYS	2.6
2	C	248	ILE	2.5
1	B	150	VAL	2.5
3	D	184	LEU	2.5
2	C	193	LYS	2.5
2	C	195	THR	2.5
1	B	65	THR	2.5
5	F	520	SER	2.5
5	F	527	LEU	2.5
2	C	224	VAL	2.4
1	B	48	GLY	2.4
3	D	956	GLY	2.4
3	D	958	THR	2.4
1	B	152	ASN	2.4
2	C	263	GLU	2.4
1	B	151	GLN	2.4
2	C	234	VAL	2.4
4	E	76	LEU	2.4
3	D	932	GLU	2.3
1	B	160	GLY	2.3
1	B	93	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	95	MET	2.3
1	A	221	LEU	2.3
2	C	223	GLY	2.3
3	D	3	ASP	2.3
1	B	134	LEU	2.3
1	B	66	VAL	2.3
1	A	224	GLU	2.3
2	C	828	LYS	2.3
1	B	118	VAL	2.3
2	C	258	MET	2.2
2	C	216	VAL	2.2
5	F	496	TYR	2.2
1	B	97	LEU	2.2
3	D	931	ASP	2.2
5	F	485	GLN	2.2
3	D	903	GLU	2.2
2	C	249	VAL	2.2
1	B	117	THR	2.2
5	F	389	ASP	2.2
1	B	7	PRO	2.2
5	F	503	ILE	2.2
3	D	959	GLN	2.2
3	D	1093	ASP	2.2
2	C	215	ASP	2.1
2	C	810	GLY	2.1
1	B	136	VAL	2.1
3	D	911	ILE	2.1
3	D	910	LEU	2.1
5	F	505	GLN	2.1
2	C	214	PHE	2.1
2	C	824	ILE	2.1
5	F	477	LEU	2.1
1	B	67	PRO	2.1
1	B	138	LEU	2.1
2	C	257	ILE	2.1
5	F	465	ASP	2.1
2	C	813	GLU	2.1
3	D	1091	HIS	2.1
2	C	261	THR	2.1
5	F	275	ALA	2.1
2	C	247	GLN	2.1
2	C	407	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	225	LEU	2.0
2	C	200	HIS	2.0
3	D	927	THR	2.0
2	C	243	TRP	2.0
3	D	905	ALA	2.0
1	B	116	VAL	2.0
5	F	475	VAL	2.0
2	C	196	ASP	2.0
5	F	517	PRO	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

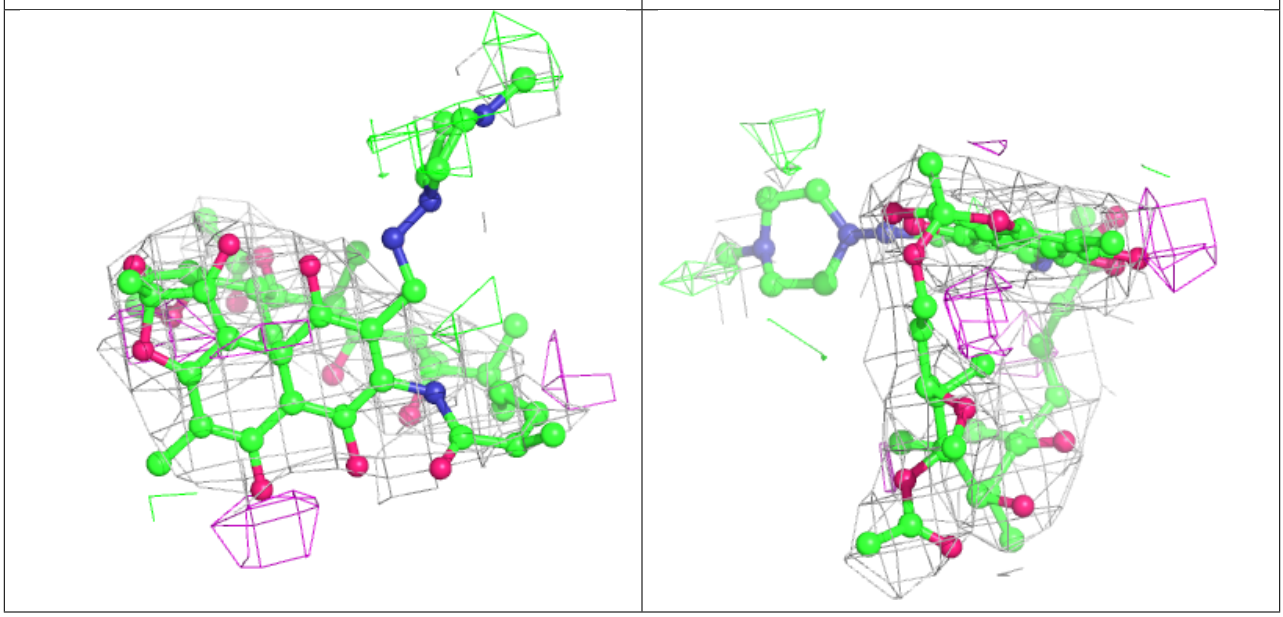
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
9	RFP	C	1201	59/59	0.94	0.27	8,26,177,177	0
11	MG	D	1403	1/1	0.94	0.27	7,7,7,7	0
10	ZN	D	1401	1/1	0.96	0.06	29,29,29,29	0
10	ZN	D	1402	1/1	0.96	0.07	35,35,35,35	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 RFP C 1201:

$2mF_o$-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

There are no such residues in this entry.