Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 01:19 PM EST

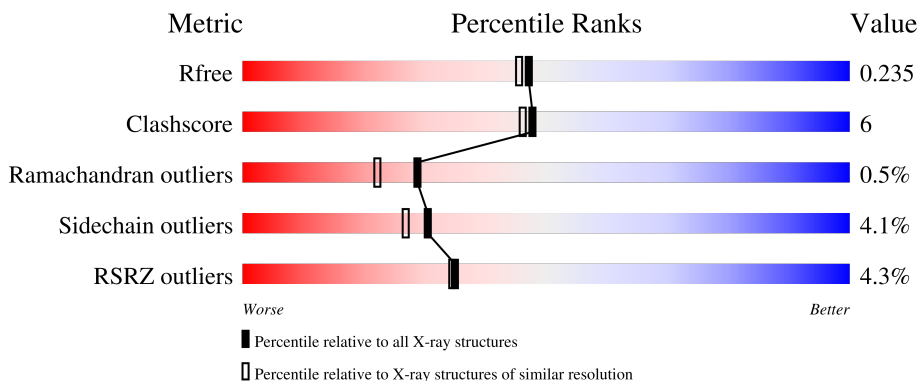|		
PDB ID	:	4FF4
Title	:	N4 mini-vRNAP transcription initiation complex, 4 min after soaking GTP, ATP and Mn
Authors	:	Murakami, K.S.
Deposited on	:	2012-05-31
Resolution	:	2.03 Å(reported)

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.03 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	Percentile Ranks	Value
Rfree		0.235
Clashscore		6
Ramachandran outliers		0.5%
Sidechain outliers		4.1%
RSRZ outliers		4.3%

Worse ▬▬▬ *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1118	4% / 84% 12% ••
1	B	1118	5% / 81% 14% ••
2	C	36	47% 8% 44%
2	D	36	44% 8% • 44%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 18998 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total 8454	C 5306	N 1435	O 1672	S 41	0	0	0
1	B	1095	Total 8454	C 5306	N 1435	O 1672	S 41	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP Q859P9
A	-10	GLY	-	expression tag	UNP Q859P9
A	-9	GLY	-	expression tag	UNP Q859P9
A	-8	SER	-	expression tag	UNP Q859P9
A	-7	HIS	-	expression tag	UNP Q859P9
A	-6	HIS	-	expression tag	UNP Q859P9
A	-5	HIS	-	expression tag	UNP Q859P9
A	-4	HIS	-	expression tag	UNP Q859P9
A	-3	HIS	-	expression tag	UNP Q859P9
A	-2	HIS	-	expression tag	UNP Q859P9
A	-1	ARG	-	expression tag	UNP Q859P9
A	0	SER	-	expression tag	UNP Q859P9
B	-11	MET	-	expression tag	UNP Q859P9
B	-10	GLY	-	expression tag	UNP Q859P9
B	-9	GLY	-	expression tag	UNP Q859P9
B	-8	SER	-	expression tag	UNP Q859P9
B	-7	HIS	-	expression tag	UNP Q859P9
B	-6	HIS	-	expression tag	UNP Q859P9
B	-5	HIS	-	expression tag	UNP Q859P9
B	-4	HIS	-	expression tag	UNP Q859P9
B	-3	HIS	-	expression tag	UNP Q859P9
B	-2	HIS	-	expression tag	UNP Q859P9
B	-1	ARG	-	expression tag	UNP Q859P9
B	0	SER	-	expression tag	UNP Q859P9

• Molecule 2 is a DNA chain called Bacteriophage N4 P2 promoter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			
2	D	20	Total	C	N	O	P	0	0	0
			413	196	80	117	20			

• Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).
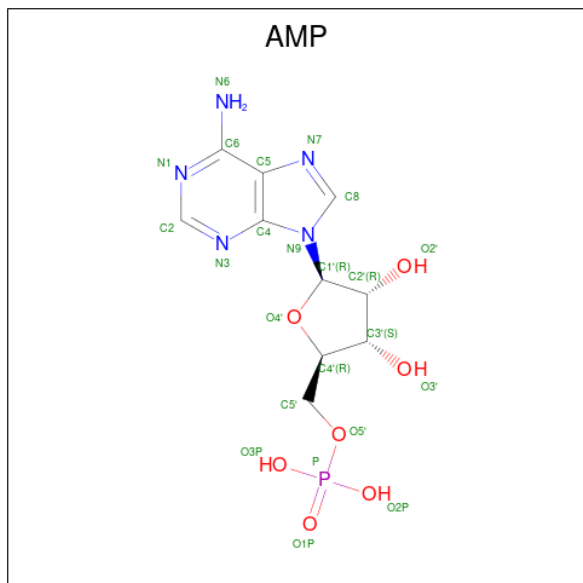
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

• Molecule 4 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: $H_2O_7P_2$).
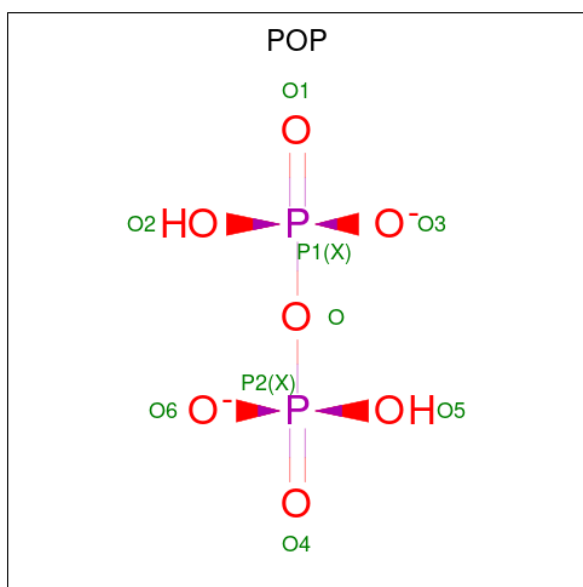
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 9	O 7	P 2	0	0

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Mn 1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
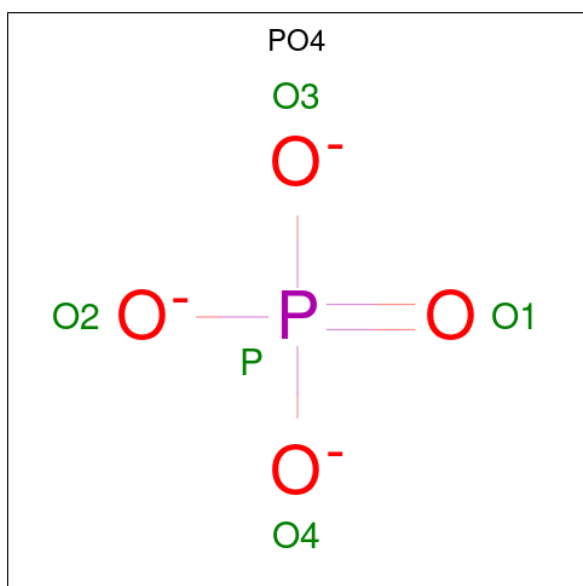
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 5	O 4	P 1	0	0
6	B	1	Total 5	O 4	P 1	0	0

• Molecule 7 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: 5GP) (formula: $C_{10}H_{14}N_5O_8P$).
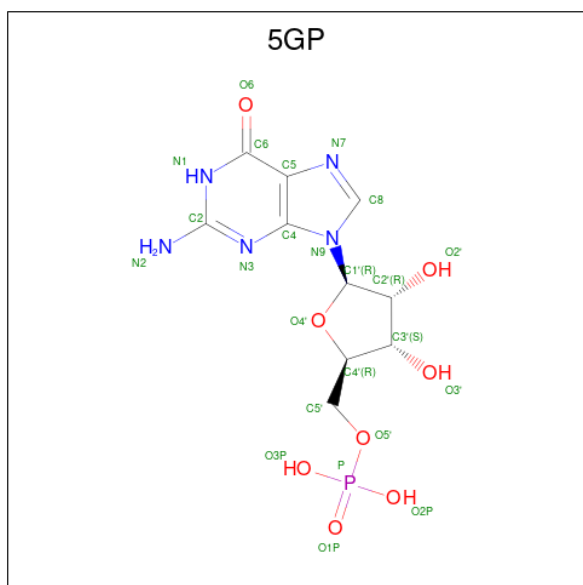
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total 24	C 10	N 5	O 8	P 1	0	0

• Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	546	Total 546	O 546	0	0
8	C	39	Total 39	O 39	0	0
8	B	572	Total 572	O 572	0	0
8	D	41	Total 41	O 41	0	0

3 Residue-property plots ⓘ

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

- Molecule 1: Virion RNA polymerase

Chain A:

- Molecule 1: Virion RNA polymerase

Chain B:

M570 K597 H602 R603 N608 N609 D610 L611 Y612 M620 E621 K625 L626 R627 S628 N629 N633 M634 P635 L649 I654 L664 K665 R666 N671 P672 L673 T674 I675 T676 I677 S680 R683 T694 V704 L705 K706 A707 R708 A709 K710 D711 P712 N713 I714

S715 M718 A719 M720 F721 G722 K723 Q724 A725 A726 S727 E728 A729 H730 E733 L734 R737 K740 T744 K752 R753 K754 T764 G765 A766 K767 G768 K769 I770 N771 P772 K773 T774 Y775 T776 I777 K778 G779 E780 Q781 L782 K783 Q786 E787 I801 L816 M830 F831 K832

Q833 R834 K838 K842 W848 F853 L854 A870 E886 N898 L899 V905 Y910 I920 A942 P943 N958 R965 W975 V983 K989 D995 K998 L1004 E1013 Y1014 D1015 Q1016 R1017 E1018 N1019 I1025 L1031 L1036 L1041

K1048 V1049 L1050 L1055 Q1059 M1060 A1061 A1062 K1072 N1088 R1092 L1095 E1096 A1097 R1098 K1099 Q1100 LYS VAL ALA LYS ALA ARG

• Molecule 2: Bacteriophage N4 P2 promoter

Chain C:
47%　　　8%　　　44%

DT DG DC DC DT DC DC DC DA DG DG DC DA T3 A8 A11 T20 T21 C22 DT DC

• Molecule 2: Bacteriophage N4 P2 promoter

Chain D:
44%　　　8%　　•　　44%

DT DG DC DC DT DC DC DC DA DG DG DC DA T3 A8 A11 G15 G16 C22 DT DT DC

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	82.40Å 111.78Å 276.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.87 – 2.03 43.87 – 2.03	Depositor EDS
% Data completeness (in resolution range)	94.1 (43.87-2.03) 90.6 (43.87-2.03)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.03Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.191 , 0.239 0.186 , 0.235	Depositor DCC
R_{free} test set	2000 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18998	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: AMP, PO4, MN, 5GP, POP

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	0.31	0/8583	0.48	1/11609 (0.0%)
1	B	0.31	0/8583	0.48	1/11609 (0.0%)
2	C	0.56	0/464	1.18	0/714
2	D	0.57	0/464	1.17	1/714 (0.1%)
All	All	0.33	0/18094	0.54	3/24646 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	444	LEU	CA-CB-CG	7.32	132.14	115.30
1	B	444	LEU	CA-CB-CG	6.14	129.42	115.30
2	D	15	DG	O4'-C1'-N9	-5.08	104.44	108.00

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	8454	0	8479	97	0
1	B	8454	0	8479	118	0
2	C	413	0	225	3	0
2	D	413	0	225	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	22	0	12	1	0
4	A	9	0	0	1	0
5	A	1	0	0	0	0
6	A	5	0	0	1	0
6	B	5	0	0	1	0
7	C	24	0	11	0	0
8	A	546	0	0	13	0
8	B	572	0	0	17	0
8	C	39	0	0	1	0
8	D	41	0	0	0	0
All	All	18998	0	17431	216	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 (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:HIS:ND1	6:B:1201:PO4:O2	2.10	0.81
1:A:767:LYS:HA	1:A:767:LYS:NZ	1.95	0.81
1:A:861:ASP:OD2	8:A:1625:HOH:O	2.02	0.76
1:A:6:GLU:N	8:A:1361:HOH:O	2.18	0.76
1:A:393:GLN:HG3	1:A:431:TYR:CD2	2.21	0.75
1:B:1018:GLU:HG3	1:B:1019:ASN:H	1.52	0.75
1:B:228:LEU:HD12	1:B:232:LYS:HD2	1.69	0.75
1:A:844:LYS:NZ	8:A:1717:HOH:O	2.20	0.74
1:B:1017:ARG:O	1:B:1019:ASN:N	2.20	0.74
1:A:228:LEU:HD12	1:A:232:LYS:HD2	1.70	0.73
1:B:1072:LYS:HA	1:B:1072:LYS:HE2	1.72	0.71
1:B:402:ARG:HA	1:B:408:ILE:HG22	1.71	0.71
1:B:610:ASP:OD2	1:B:666:ARG:NH1	2.25	0.70
1:A:999:LEU:HB2	1:A:1004:LEU:HD23	1.73	0.70
1:A:617:ASN:HA	1:A:620:MET:HE2	1.74	0.70
1:A:191:GLU:HG3	1:A:375:ASN:HB3	1.74	0.69
1:B:612:TYR:HD1	1:B:666:ARG:NH1	1.89	0.69
1:B:570:MET:HE2	1:B:975:TRP:HB3	1.75	0.69
1:A:190:PRO:HG2	1:A:262:ILE:HG23	1.74	0.69
1:B:649:LEU:HD13	1:B:737:ARG:NH2	2.08	0.69
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.75	0.68
1:A:1018:GLU:HG3	1:A:1019:ASN:H	1.60	0.67
1:B:711:ASP:C	1:B:713:ASN:H	1.98	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:ARG:O	1:A:1019:ASN:N	2.28	0.67
2:C:20:DT:O4	8:C:217:HOH:O	2.12	0.66
1:A:612:TYR:HD1	1:A:666:ARG:NH1	1.92	0.66
1:A:328:GLN:HG2	1:A:419:MET:HE3	1.77	0.66
1:B:711:ASP:O	1:B:713:ASN:N	2.29	0.66
1:B:393:GLN:HG3	1:B:431:TYR:CD2	2.30	0.65
1:B:694:THR:HG22	1:B:777:ILE:HD12	1.78	0.65
1:A:1072:LYS:HA	1:A:1072:LYS:HE2	1.79	0.65
1:B:870:ALA:HB2	1:B:989:LYS:HD3	1.79	0.64
1:B:496:LYS:NZ	8:B:1687:HOH:O	2.31	0.64
1:A:886:GLU:O	2:C:8:DA:H4'	1.98	0.64
1:B:783:LYS:O	1:B:787:GLU:HG2	1.97	0.63
1:B:958:ASN:ND2	8:B:1799:HOH:O	2.32	0.63
1:B:355:LYS:HD2	1:B:388:GLU:HG3	1.80	0.62
1:B:191:GLU:HG3	1:B:375:ASN:HB3	1.82	0.62
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.82	0.61
1:A:767:LYS:HA	1:A:767:LYS:HZ3	1.64	0.60
1:B:764:THR:OG1	1:B:765:GLY:N	2.31	0.60
1:B:740:LYS:O	1:B:744:THR:HG22	2.02	0.59
1:B:332:LEU:O	1:B:336:GLN:HG3	2.02	0.59
1:A:767:LYS:HA	1:A:767:LYS:HZ2	1.67	0.58
1:B:771:ASN:OD1	1:B:774:THR:OG1	2.18	0.58
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.84	0.58
1:A:714:ILE:HD11	1:A:718:MET:HB3	1.86	0.58
1:B:1048:LYS:HD2	1:B:1098:ARG:HH21	1.69	0.57
1:B:830:MET:O	1:B:834:ARG:HG3	2.04	0.57
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.87	0.57
1:B:710:LYS:O	1:B:711:ASP:HB3	2.04	0.56
1:B:597:LYS:HE2	1:B:602:HIS:HB2	1.87	0.56
1:A:1002:GLU:OE1	1:A:1002:GLU:N	2.29	0.56
1:B:257:VAL:HG12	1:B:259:MET:HE3	1.87	0.56
1:A:965:ARG:HD2	8:A:1702:HOH:O	2.05	0.56
1:B:190:PRO:HG2	1:B:262:ILE:HG23	1.88	0.56
1:B:621:GLU:OE1	8:B:1730:HOH:O	2.17	0.56
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.06	0.56
1:B:158:ALA:HB1	1:B:213:LYS:HG3	1.88	0.55
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.88	0.55
1:B:421:ARG:HG3	8:B:1312:HOH:O	2.05	0.55
1:B:965:ARG:NH2	8:B:1724:HOH:O	2.35	0.55
1:A:47:ARG:NH1	8:A:1533:HOH:O	2.41	0.54
1:B:673:LEU:HD22	1:B:801:ILE:HG12	1.89	0.54

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:LYS:HB3	1:A:848:TRP:CD2	2.43	0.54
1:A:1004:LEU:HD13	1:A:1025:ILE:HG13	1.90	0.54
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.89	0.53
1:A:612:TYR:CD1	1:A:666:ARG:NH1	2.74	0.53
1:B:259:MET:HA	1:B:259:MET:HE2	1.89	0.53
1:B:842:LYS:NZ	8:B:1385:HOH:O	2.25	0.53
1:B:1018:GLU:HG3	1:B:1019:ASN:N	2.23	0.53
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.89	0.53
1:B:257:VAL:HG12	1:B:259:MET:CE	2.39	0.53
1:B:727:SER:OG	1:B:730:HIS:HB2	2.09	0.53
1:B:88:ARG:HD3	1:B:282:ASP:OD1	2.10	0.52
1:A:488:THR:O	1:A:492:GLU:HG2	2.09	0.52
1:B:114:LYS:NZ	2:D:15:DG:N7	2.56	0.52
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.09	0.52
1:A:257:VAL:HG12	1:A:259:MET:CE	2.41	0.51
1:B:625:LYS:O	1:B:629:ASN:ND2	2.43	0.51
1:B:965:ARG:NE	8:B:1724:HOH:O	2.36	0.51
1:B:52:GLU:H	1:B:52:GLU:CD	2.14	0.51
1:A:274:THR:HG23	8:A:1387:HOH:O	2.09	0.51
1:B:402:ARG:HA	1:B:408:ILE:CG2	2.40	0.51
1:A:95:HIS:HA	1:B:248:GLU:O	2.11	0.51
1:A:377:ALA:O	1:A:381:GLU:HG3	2.11	0.51
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.93	0.51
1:B:182:THR:HB	1:B:259:MET:SD	2.51	0.51
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.44	0.51
1:A:471:LEU:O	1:A:526:ARG:HD3	2.11	0.51
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.58	0.51
1:A:190:PRO:HG2	1:A:262:ILE:CG2	2.40	0.50
1:B:718:MET:HE3	1:B:728:GLU:HA	1.94	0.50
1:B:677:ILE:O	1:B:920:ILE:HG21	2.11	0.50
1:A:764:THR:O	1:A:764:THR:OG1	2.29	0.50
1:B:777:ILE:HG22	1:B:782:LEU:HG	1.94	0.49
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.94	0.49
1:A:753:ARG:NH2	8:A:1796:HOH:O	2.45	0.49
1:B:965:ARG:NH1	8:B:1673:HOH:O	2.32	0.49
1:B:395:PHE:O	1:B:399:GLU:HG2	2.13	0.49
1:A:463:PHE:HA	1:A:957:LEU:HD13	1.95	0.49
1:A:821:GLN:O	1:A:825:VAL:HG23	2.13	0.49
1:A:675:ILE:HD11	1:A:685:ILE:HG12	1.94	0.48
1:B:229:GLY:O	1:B:233:GLY:HA3	2.13	0.48
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:TYR:OH	1:A:1051:ASP:OD1	2.27	0.48
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.14	0.48
1:B:675:ILE:O	1:B:680:SER:HB3	2.13	0.48
1:A:1018:GLU:HG3	1:A:1019:ASN:N	2.26	0.48
1:B:886:GLU:O	2:D:8:DA:H4'	2.13	0.48
1:A:368:ASN:O	1:A:370:GLU:N	2.47	0.47
1:A:228:LEU:HD23	1:A:854:LEU:O	2.14	0.47
1:A:694:THR:HG22	1:A:777:ILE:HD12	1.97	0.47
1:A:1016:GLN:O	1:A:1020:ALA:HB2	2.15	0.47
1:B:72:THR:O	1:B:74:LYS:HG2	2.14	0.47
1:A:499:ILE:HD12	1:A:538:TYR:HD2	1.80	0.47
1:A:1092:ARG:HH11	1:A:1092:ARG:HG2	1.80	0.47
1:B:488:THR:O	1:B:492:GLU:HG2	2.15	0.47
1:B:321:ALA:HB2	1:B:910:TYR:HE1	1.80	0.47
1:B:722:GLY:N	8:B:1796:HOH:O	2.36	0.47
1:A:33:TYR:OH	1:A:128:ARG:CZ	2.63	0.47
1:B:710:LYS:HB3	1:B:710:LYS:HE2	1.67	0.47
1:A:1004:LEU:CD1	1:A:1025:ILE:HG13	2.44	0.46
1:B:1088:ASN:O	1:B:1092:ARG:HG3	2.16	0.46
1:B:725:ALA:HB3	8:B:1744:HOH:O	2.14	0.46
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.51	0.46
1:B:279:ASP:HB3	1:B:281:PHE:CE1	2.51	0.46
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.16	0.46
1:A:93:MET:HA	1:A:93:MET:HE2	1.98	0.46
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.98	0.46
1:A:554:LEU:HD23	1:A:957:LEU:HD11	1.98	0.46
1:B:779:GLY:O	1:B:783:LYS:HG3	2.16	0.46
1:A:597:LYS:HE2	1:A:602:HIS:HB2	1.97	0.45
1:B:259:MET:HE2	1:B:262:ILE:HD12	1.98	0.45
1:B:832:LYS:HG3	8:B:1786:HOH:O	2.15	0.45
1:B:995:ASP:OD1	1:B:998:LYS:HG3	2.15	0.45
1:B:113:THR:HG22	1:B:114:LYS:HG3	1.98	0.45
1:B:328:GLN:HG2	1:B:419:MET:HE3	1.98	0.45
1:B:214:ILE:HD11	1:B:242:ILE:HD12	1.99	0.45
1:B:718:MET:CE	1:B:728:GLU:HA	2.47	0.45
1:A:272:LEU:HD12	1:A:272:LEU:HA	1.81	0.45
1:A:619:LEU:HD12	1:A:619:LEU:O	2.17	0.45
1:A:642:SER:OG	1:A:740:LYS:NZ	2.50	0.45
1:B:710:LYS:O	1:B:711:ASP:CB	2.65	0.45
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.65	0.45
1:B:694:THR:HG22	1:B:777:ILE:CD1	2.45	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1072:LYS:HE2	1:B:1072:LYS:CA	2.44	0.45
1:A:328:GLN:HG2	1:A:419:MET:CE	2.45	0.45
1:B:1048:LYS:HD2	1:B:1098:ARG:NH2	2.31	0.45
1:A:101:ASP:OD1	1:B:109:LYS:HE3	2.18	0.44
1:B:489:LYS:NZ	8:B:1606:HOH:O	2.50	0.44
1:A:397:VAL:O	1:A:401:VAL:HG23	2.17	0.44
1:B:654:ILE:HD13	1:B:664:LEU:HD22	1.99	0.44
1:B:708:ARG:HA	1:B:714:ILE:HG21	1.98	0.44
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.32	0.44
1:B:269:THR:O	2:D:11:DA:H5'	2.18	0.44
1:A:616:THR:CG2	1:A:664:LEU:HB2	2.48	0.43
1:A:706:LYS:HB2	1:A:706:LYS:HE3	1.68	0.43
1:A:791:HIS:ND1	1:A:795:GLU:OE2	2.50	0.43
1:B:259:MET:CE	1:B:262:ILE:HD12	2.48	0.43
1:B:633:ASN:OD1	1:B:635:PRO:HD2	2.18	0.43
1:B:1004:LEU:CD1	1:B:1025:ILE:HG13	2.48	0.43
1:B:394:LEU:O	1:B:398:ILE:HG12	2.19	0.43
1:B:942:ALA:HA	1:B:943:PRO:HD3	1.89	0.43
1:B:20:VAL:HG23	1:B:138:VAL:O	2.18	0.43
3:A:1201:AMP:P	4:A:1202:POP:O3	2.77	0.43
1:B:673:LEU:HD13	1:B:673:LEU:O	2.19	0.43
1:B:853:PHE:CG	1:B:854:LEU:N	2.87	0.43
1:B:995:ASP:CG	1:B:998:LYS:HG3	2.38	0.43
1:A:476:HIS:ND1	6:A:1204:PO4:O1	2.34	0.43
1:B:627:ARG:NE	8:B:1716:HOH:O	2.50	0.43
1:B:565:PRO:HG3	1:B:673:LEU:HD12	2.01	0.43
1:A:633:ASN:OD1	1:A:635:PRO:HD2	2.19	0.42
1:B:362:MET:HE1	1:B:528:SER:HA	1.99	0.42
1:B:1017:ARG:O	1:B:1018:GLU:C	2.58	0.42
1:A:279:ASP:HB3	1:A:281:PHE:CE1	2.53	0.42
1:A:764:THR:HG23	8:A:1596:HOH:O	2.20	0.42
1:B:816:LEU:O	1:B:816:LEU:HD12	2.20	0.42
1:A:671:ASN:HB3	1:A:672:PRO:HD3	2.02	0.42
1:B:721:PHE:O	8:B:1744:HOH:O	2.21	0.42
1:A:368:ASN:C	1:A:370:GLU:H	2.23	0.42
1:B:13:ASP:HB2	8:B:1671:HOH:O	2.18	0.42
1:B:438:LEU:HD23	1:B:438:LEU:C	2.40	0.42
1:A:189:LEU:HA	1:A:190:PRO:HD3	1.93	0.42
1:A:1050:LEU:HD12	1:A:1050:LEU:HA	1.87	0.42
1:B:440:ARG:O	1:B:444:LEU:HD13	2.19	0.42
1:A:1037:ARG:HG3	8:A:1811:HOH:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1092:ARG:HG2	1:A:1092:ARG:NH1	2.35	0.41
1:A:259:MET:HA	1:A:259:MET:HE2	2.02	0.41
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.46	0.41
1:A:1012:LEU:O	1:A:1017:ARG:NH1	2.51	0.41
1:B:75:GLU:HG3	1:B:76:THR:N	2.35	0.41
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.92	0.41
1:B:838:LYS:HD3	1:B:838:LYS:HA	1.78	0.41
1:A:44:GLN:NE2	8:A:1458:HOH:O	2.24	0.41
1:A:210:LEU:HB3	1:A:239:ALA:HB1	2.03	0.41
1:A:393:GLN:HG2	8:A:1783:HOH:O	2.20	0.41
1:B:474:LYS:HD3	1:B:474:LYS:HA	1.90	0.41
1:A:864:ALA:HB3	8:A:1826:HOH:O	2.21	0.41
1:A:965:ARG:NH2	8:A:1488:HOH:O	2.37	0.41
1:A:1015:ASP:CG	1:A:1016:GLN:N	2.74	0.41
1:A:177:ASP:O	1:A:181:ILE:HG13	2.21	0.41
1:A:634:MET:N	1:A:635:PRO:CD	2.84	0.41
1:A:677:ILE:O	1:A:920:ILE:HG21	2.21	0.41
1:A:794:VAL:O	1:A:798:ARG:HG2	2.20	0.41
1:B:241:GLU:OE2	1:B:898:ASN:HB2	2.21	0.41
1:B:965:ARG:CZ	8:B:1724:HOH:O	2.69	0.41
1:A:269:THR:O	2:C:11:DA:H5'	2.21	0.41
1:B:200:GLY:HA2	1:B:274:THR:HG22	2.01	0.40
1:B:683:ARG:HG2	1:B:786:GLN:HE21	1.86	0.40
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.56	0.40
1:B:733:GLU:HG2	1:B:734:LEU:N	2.34	0.40
1:A:72:THR:O	1:A:74:LYS:HE3	2.21	0.40
1:B:173:LYS:NZ	8:B:1547:HOH:O	2.37	0.40
2:D:15:DG:H2"	2:D:16:DG:C8	2.57	0.40
1:B:620:MET:HG3	1:B:664:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3　Torsion angles ⓘ

5.3.1　Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1093/1118 (98%)	1065 (97%)	23 (2%)	5 (0%)	29	22
1	B	1093/1118 (98%)	1057 (97%)	30 (3%)	6 (0%)	29	22
All	All	2186/2236 (98%)	2122 (97%)	53 (2%)	11 (0%)	29	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	B	711	ASP
1	B	1018	GLU
1	A	369	LYS
1	A	779	GLY
1	A	1017	ARG
1	A	1062	ALA
1	B	1017	ARG
1	B	1062	ALA
1	B	712	PRO
1	B	779	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	916/935 (98%)	882 (96%)	34 (4%)	34	31
1	B	916/935 (98%)	874 (95%)	42 (5%)	27	22
All	All	1832/1870 (98%)	1756 (96%)	76 (4%)	30	27

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	70	LEU
1	A	163	ARG
1	A	210	LEU
1	A	261	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	LEU
1	A	281	PHE
1	A	284	ILE
1	A	406	GLU
1	A	419	MET
1	A	444	LEU
1	A	471	LEU
1	A	472	ASP
1	A	517	ASP
1	A	520	ASN
1	A	525	ASP
1	A	541	TYR
1	A	649	LEU
1	A	673	LEU
1	A	691	SER
1	A	764	THR
1	A	782	LEU
1	A	838	LYS
1	A	886	GLU
1	A	908	SER
1	A	936	LEU
1	A	1004	LEU
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU
1	A	1059	GLN
1	A	1093	GLU
1	A	1099	LYS
1	B	52	GLU
1	B	70	LEU
1	B	88	ARG
1	B	122	GLN
1	B	163	ARG
1	B	216	SER
1	B	228	LEU
1	B	261	GLU
1	B	272	LEU
1	B	281	PHE
1	B	372	LEU
1	B	390	SER
1	B	419	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	444	LEU
1	B	471	LEU
1	B	472	ASP
1	B	489	LYS
1	B	517	ASP
1	B	520	ASN
1	B	525	ASP
1	B	603	ARG
1	B	649	LEU
1	B	673	LEU
1	B	714	ILE
1	B	715	SER
1	B	718	MET
1	B	733	GLU
1	B	734	LEU
1	B	752	LYS
1	B	764	THR
1	B	767	LYS
1	B	838	LYS
1	B	886	GLU
1	B	1004	LEU
1	B	1014	TYR
1	B	1031	LEU
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1055	LEU
1	B	1059	GLN
1	B	1099	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	506	ASN
1	B	520	ASN
1	B	671	ASN
1	B	863	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6   Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#|Z| > 2$
6	PO4	B	1201	-	4,4,4	0.84	0	6,6,6	0.48	0
4	POP	A	1202	5	6,8,8	0.67	0	13,13,13	1.24	3 (23%)
6	PO4	A	1204	-	4,4,4	0.91	0	6,6,6	0.66	0
7	5GP	C	101	3	22,26,26	1.16	2 (9%)	26,40,40	1.29	4 (15%)
3	AMP	A	1201	7	18,24,25	0.69	0	18,35,38	0.87	0

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
3	AMP	A	1201	7	-	0/3/25/26	0/3/3/3
7	5GP	C	101	3	-	0/6/26/26	0/3/3/3
4	POP	A	1202	5	-	2/6/6/6	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	101	5GP	C5-C6	-3.68	1.39	1.47
7	C	101	5GP	C6-N1	-2.00	1.34	1.37

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	101	5GP	O3P-P-O5'	-3.02	98.71	106.73
7	C	101	5GP	C5-C6-N1	2.87	119.01	113.95
4	A	1202	POP	O5-P2-O	2.35	112.53	104.64
7	C	101	5GP	C8-N7-C5	2.34	107.45	102.99
7	C	101	5GP	C2-N1-C6	-2.18	121.07	125.10
4	A	1202	POP	P2-O-P1	-2.15	125.44	132.83
4	A	1202	POP	O2-P1-O	2.05	111.51	104.64

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1202	POP	P1-O-P2-O6
4	A	1202	POP	P1-O-P2-O4

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1201	PO4	1	0
4	A	1202	POP	1	0
6	A	1204	PO4	1	0
3	A	1201	AMP	1	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 5GP C 101

Bond lengths

Bond angles

Torsions

Rings
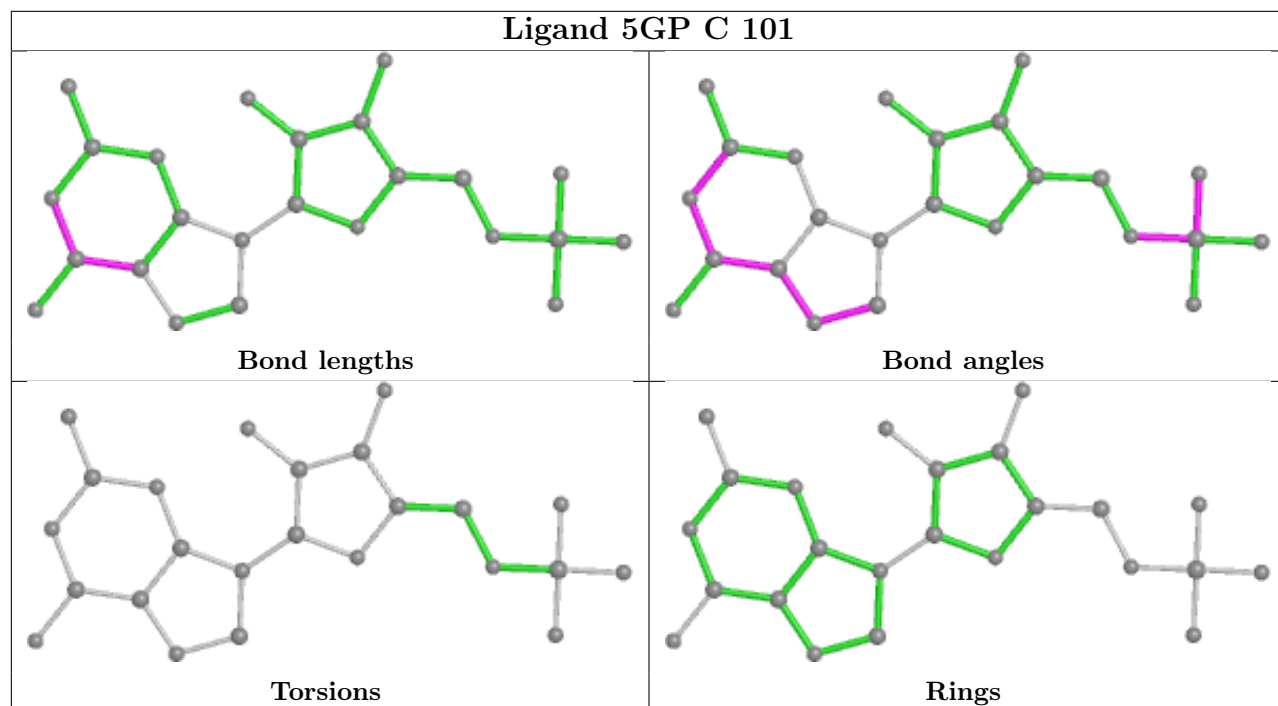
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1095/1118 (97%)	-0.01	41 (3%)	41	41	16, 34, 72, 106	0
1	B	1095/1118 (97%)	0.10	55 (5%)	28	28	15, 33, 75, 147	0
2	C	20/36 (55%)	-0.39	0	100	100	34, 41, 70, 71	0
2	D	20/36 (55%)	-0.37	0	100	100	28, 41, 69, 96	0
All	All	2230/2308 (96%)	0.04	96 (4%)	35	34	15, 33, 72, 147	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	ALA	15.2
1	B	1018	GLU	9.1
1	B	1099	LYS	8.0
1	B	1100	GLN	6.7
1	A	8	LEU	6.0
1	B	770	ILE	5.9
1	B	1019	ASN	5.5
1	B	727	SER	4.9
1	B	725	ALA	4.9
1	B	707	ALA	4.9
1	B	708	ARG	4.9
1	A	264	PRO	4.5
1	B	722	GLY	4.5
1	B	728	GLU	4.3
1	B	713	ASN	4.2
1	B	767	LYS	4.1
1	B	27	ALA	4.0
1	B	723	LYS	4.0
1	A	1018	GLU	3.9
1	B	1014	TYR	3.9
1	B	371	LEU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	658	GLU	3.7
1	A	262	ILE	3.7
1	B	6	GLU	3.7
1	B	766	ALA	3.6
1	A	725	ALA	3.5
1	A	713	ASN	3.5
1	B	730	HIS	3.5
1	A	708	ARG	3.3
1	B	262	ILE	3.3
1	B	191	GLU	3.2
1	B	780	GLU	3.2
1	A	261	GLU	3.2
1	B	1096	GLU	3.2
1	B	704	VAL	3.1
1	A	1099	LYS	3.1
1	B	260	SER	3.1
1	A	371	LEU	3.1
1	B	712	PRO	3.0
1	A	726	ALA	3.0
1	B	729	ALA	3.0
1	B	718	MET	2.9
1	A	28	GLU	2.8
1	B	769	LYS	2.8
1	A	265	ASP	2.8
1	B	1098	ARG	2.8
1	B	265	ASP	2.7
1	B	724	GLN	2.7
1	B	754	LYS	2.7
1	A	188	LEU	2.7
1	A	709	ALA	2.7
1	B	1015	ASP	2.7
1	A	258	ASP	2.7
1	B	710	LYS	2.7
1	B	264	PRO	2.7
1	B	764	THR	2.7
1	A	7	GLU	2.6
1	B	8	LEU	2.6
1	A	780	GLU	2.4
1	B	772	PRO	2.4
1	B	42	GLU	2.4
1	A	711	ASP	2.4
1	A	260	SER	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	754	LYS	2.4
1	A	844	LYS	2.4
1	A	1005	GLU	2.4
1	B	28	GLU	2.3
1	A	910	TYR	2.3
1	A	6	GLU	2.3
1	A	40	LEU	2.3
1	A	767	LYS	2.3
1	A	1098	ARG	2.3
1	B	26	LYS	2.3
1	B	711	ASP	2.3
1	B	752	LYS	2.2
1	B	775	TYR	2.2
1	B	899	LEU	2.2
1	B	706	LYS	2.2
1	A	267	LYS	2.2
1	B	1095	LEU	2.2
1	A	753	ARG	2.2
1	B	1013	GLU	2.2
1	B	70	LEU	2.2
1	A	10	GLU	2.2
1	A	366	THR	2.2
1	B	263	ASP	2.1
1	A	1015	ASP	2.1
1	A	719	ALA	2.1
1	B	10	GLU	2.1
1	A	764	THR	2.1
1	A	43	GLU	2.0
1	A	710	LYS	2.0
1	A	729	ALA	2.0
1	B	719	ALA	2.0
1	A	722	GLY	2.0
1	A	1014	TYR	2.0

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

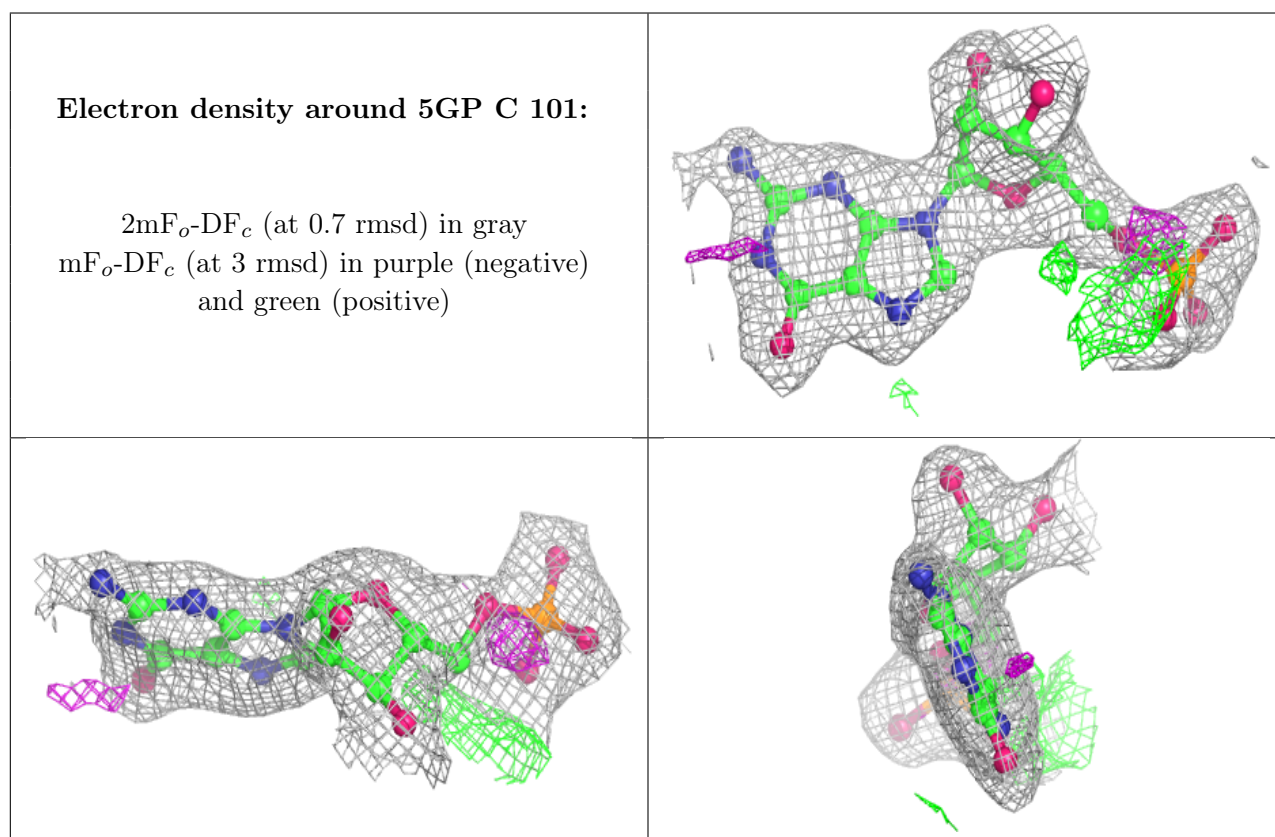There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	POP	A	1202	9/9	0.81	0.20	36,69,75,240	0
5	MN	A	1203	1/1	0.85	0.08	92,92,92,92	0
7	5GP	C	101	24/24	0.89	0.13	36,43,61,72	0
3	AMP	A	1201	22/23	0.93	0.12	33,36,53,59	0
6	PO4	B	1201	5/5	0.96	0.13	49,50,57,58	0
6	PO4	A	1204	5/5	0.97	0.13	43,47,49,53	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 5GP C 101:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.