



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2026 – 06:23 PM EDT

PDB ID : 4FF2 / pdb\_00004ff2  
Title : N4 mini-vRNAP transcription initiation complex, 2 min after soaking GTP, ATP and Mn  
Authors : Murakami, K.S.; Basu, R.S.  
Deposited on : 2012-05-30  
Resolution : 2.00 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

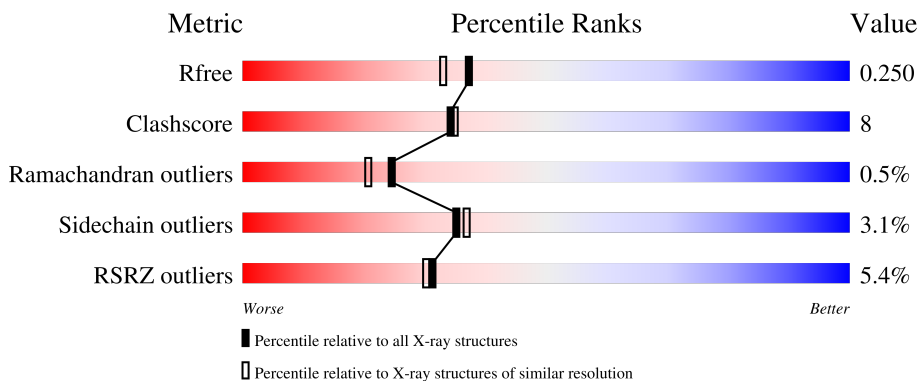
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1118	 4% 78% 19% ..
1	B	1118	 6% 80% 17% ..
2	C	36	 50% 6% 44%
2	D	36	 3% 33% 22% 44%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 18981 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
			Total	C	N	O	S			
1	A	1095	8462	5310	1436	1675	41	0	1	0
1	B	1095	8454	5306	1435	1672	41	0	0	0

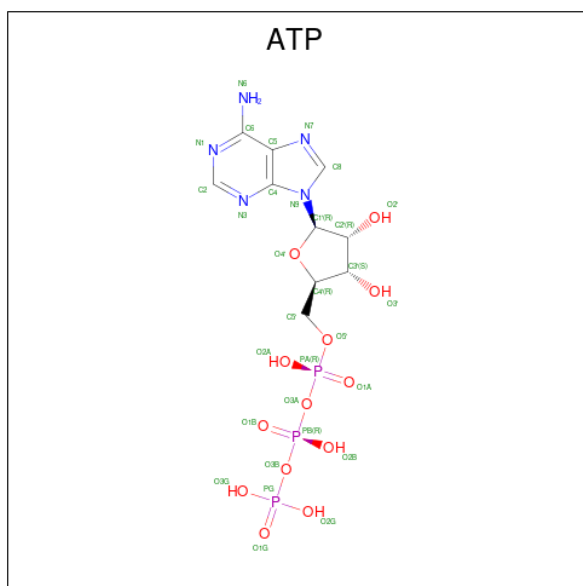
There are 24 discrepancies between the modelled and reference sequences:

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
			Total	C	N	O	P			
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-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 4 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

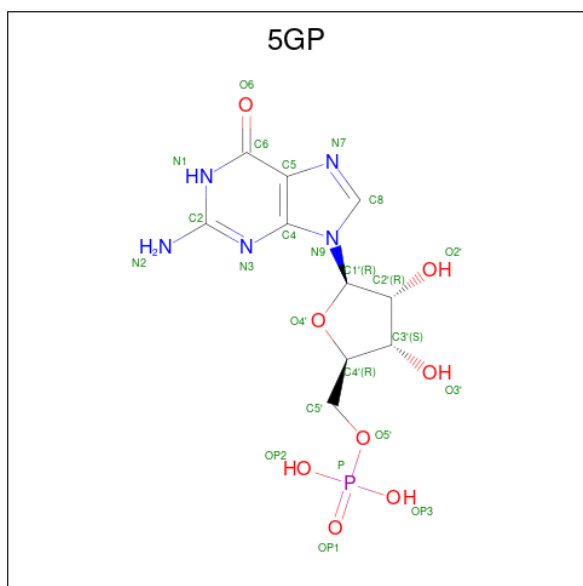
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mn		
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0

- Molecule 6 is GUANOSINE-5'-MONOPHOSPHATE (CCD ID: 5GP) (formula:  $C_{10}H_{14}N_5O_8P$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O P 24 10 5 8 1	0	0

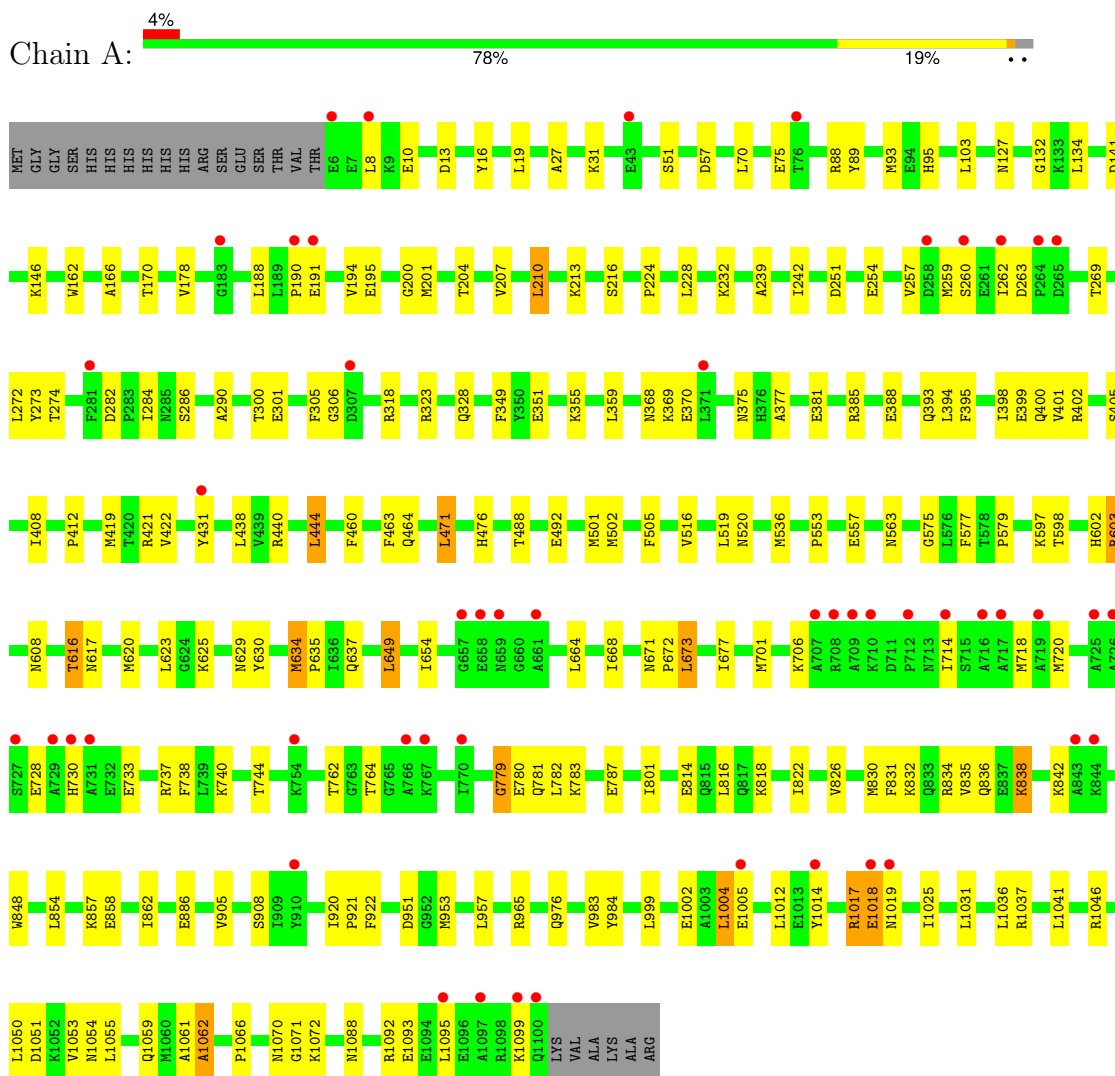
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	547	Total 547	O 547	0	0
7	C	33	Total 33	O 33	0	0
7	B	557	Total 557	O 557	0	0
7	D	36	Total 36	O 36	0	0

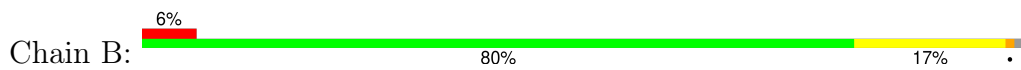
### 3 Residue-property plots [i](#)

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: Virion RNA polymerase



- Molecule 1: Virion RNA polymerase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.91Å 111.44Å 275.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.00 47.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.7 (47.67-2.00) 86.9 (47.67-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.65 (at 1.98Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.208 , 0.255 0.203 , 0.250	Depositor DCC
$R_{free}$ test set	2000 reflections (1.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	18.9	Xtrriage
Anisotropy	0.116	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	18981	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, 5GP, PO4, MN

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	0.35	0/8591	0.72	4/11620 (0.0%)
1	B	0.35	0/8583	0.72	3/11609 (0.0%)
2	C	0.16	0/464	0.66	0/714
2	D	0.17	0/464	0.66	0/714
All	All	0.35	0/18102	0.72	7/24657 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	771	ASN	CA-C-N	5.77	125.90	119.32
1	B	771	ASN	C-N-CA	5.77	125.90	119.32
1	A	563	ASN	N-CA-C	5.44	116.90	110.97
1	A	251	ASP	N-CA-C	-5.27	106.36	112.89
1	B	563	ASN	N-CA-C	5.23	116.66	111.07
1	A	263	ASP	CA-C-N	5.18	125.48	119.47
1	A	263	ASP	C-N-CA	5.18	125.48	119.47

There are no chirality outliers.

There are no planarity outliers.

### 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	A	8462	0	8482	141	0
1	B	8454	0	8479	124	0
2	C	413	0	225	2	0
2	D	413	0	225	8	0
3	A	31	0	12	0	0
4	A	1	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	1	0
6	C	24	0	12	0	0
7	A	547	0	0	9	1
7	B	557	0	0	3	1
7	C	33	0	0	0	0
7	D	36	0	0	3	0
All	All	18981	0	17435	268	1

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 8.

All (268) 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:664:LEU:HB3	1:B:668:ILE:HD11	1.40	1.03
1:B:701:MET:HE1	1:B:720:MET:HE2	1.46	0.98
1:B:1018:GLU:HG3	1:B:1019:ASN:H	1.33	0.90
1:A:228:LEU:HD12	1:A:232:LYS:HD2	1.59	0.84
1:B:191:GLU:HG3	1:B:375:ASN:HB3	1.62	0.81
1:A:306:GLY:HA2	1:A:412:PRO:HG2	1.61	0.80
1:A:191:GLU:HG3	1:A:375:ASN:HB3	1.63	0.80
1:B:603:ARG:NH1	1:B:608:ASN:OD1	2.16	0.79
1:B:991:MET:HE2	1:B:1030:SER:HB3	1.64	0.78
1:B:612:TYR:CE2	1:B:673:LEU:HD23	2.20	0.77
1:A:718:MET:HE2	1:A:728:GLU:HA	1.68	0.75
1:B:783:LYS:O	1:B:787:GLU:HG2	1.87	0.74
1:B:306:GLY:HA2	1:B:412:PRO:HG2	1.69	0.73
1:B:740:LYS:O	1:B:744:THR:HG22	1.91	0.70
1:A:351:GLU:HG3	1:A:395:PHE:CE2	2.27	0.69
1:A:976:GLN:NE2	7:A:1339:HOH:O	2.15	0.69
1:B:395:PHE:O	1:B:399:GLU:HG2	1.92	0.69
1:A:395:PHE:O	1:A:399:GLU:HG2	1.93	0.69
1:A:762:THR:HB	1:A:764:THR:HG22	1.73	0.69
1:B:612:TYR:HD1	1:B:666:ARG:NH1	1.91	0.68
1:B:393:GLN:HG3	1:B:431:TYR:CD2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:HA	1:A:620:MET:HE2	1.75	0.67
1:B:476:HIS:ND1	5:B:1201:PO4:O2	2.24	0.67
1:A:1095:LEU:HG	1:A:1099:LYS:HE3	1.76	0.67
1:B:1048:LYS:HD2	1:B:1098:ARG:HH21	1.60	0.66
1:A:625:LYS:O	1:A:629:ASN:ND2	2.28	0.65
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.78	0.65
1:A:190:PRO:HG2	1:A:262:ILE:HG23	1.77	0.65
1:A:393:GLN:HG3	1:A:431:TYR:CD2	2.33	0.64
1:A:1051:ASP:HB2	7:A:1339:HOH:O	1.98	0.64
1:B:200:GLY:HA2	1:B:274:THR:HG22	1.79	0.63
1:B:402:ARG:HA	1:B:408:ILE:HG22	1.79	0.63
1:A:1017:ARG:O	1:A:1019:ASN:N	2.32	0.63
1:A:1072:LYS:HE2	1:A:1072:LYS:HA	1.81	0.63
1:B:598:THR:HG22	1:B:1066:PRO:HD3	1.80	0.63
1:B:718:MET:HE2	1:B:728:GLU:HA	1.79	0.63
1:A:476:HIS:ND1	5:A:1203:PO4:O1	2.26	0.63
1:B:1018:GLU:HG3	1:B:1019:ASN:N	2.11	0.62
1:B:348:GLN:OE1	7:B:1727:HOH:O	2.16	0.62
1:A:200:GLY:HA2	1:A:274:THR:HG22	1.81	0.61
1:A:170:THR:HG22	1:A:201:MET:HE3	1.82	0.60
1:A:1088:ASN:O	1:A:1092:ARG:HG3	2.01	0.60
1:B:694:THR:HG22	1:B:777:ILE:HD12	1.82	0.60
1:B:984:TYR:CE1	1:B:1037:ARG:HB2	2.37	0.60
1:A:826:VAL:HG22	1:A:999:LEU:HD11	1.83	0.60
1:B:88:ARG:HD2	1:B:283:PRO:HD2	1.81	0.60
1:B:917:VAL:HG21	2:D:4:DT:H4'	1.83	0.59
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.83	0.59
1:B:1053:VAL:HG11	1:B:1075:LEU:HD12	1.84	0.59
1:B:113:THR:HG22	1:B:114:LYS:HG3	1.84	0.58
1:A:842:LYS:HB3	1:A:848:TRP:CD2	2.38	0.58
1:A:671:ASN:HB3	1:A:672:PRO:HD3	1.86	0.58
1:A:818:LYS:O	1:A:822:ILE:HG13	2.04	0.57
1:A:377:ALA:O	1:A:381:GLU:HG3	2.04	0.57
1:A:1070:ASN:HB2	7:A:1480:HOH:O	2.04	0.57
1:A:1018:GLU:HG3	1:A:1019:ASN:H	1.69	0.57
1:B:188:LEU:HD21	1:B:783:LYS:HG2	1.87	0.57
1:B:257:VAL:HG12	1:B:259:MET:CE	2.35	0.57
1:B:818:LYS:O	1:B:822:ILE:HG13	2.04	0.57
1:A:999:LEU:HB2	1:A:1004:LEU:CD2	2.35	0.57
2:D:15:DG:OP1	7:D:115:HOH:O	2.17	0.56
1:A:488:THR:O	1:A:492:GLU:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ILE:HB	1:B:235:PRO:HD3	1.87	0.56
1:A:328:GLN:HG2	1:A:419:MET:HE3	1.88	0.56
1:A:649:LEU:HD13	1:A:737:ARG:NH2	2.21	0.56
1:A:440:ARG:O	1:A:444:LEU:HD13	2.05	0.55
1:B:649:LEU:HD13	1:B:737:ARG:NH2	2.21	0.55
1:B:617:ASN:HA	1:B:620:MET:HE2	1.88	0.55
1:B:830:MET:O	1:B:834:ARG:HG3	2.05	0.55
1:B:612:TYR:HE2	1:B:673:LEU:HD23	1.71	0.55
1:B:597:LYS:HE2	1:B:602:HIS:HB2	1.89	0.54
1:A:740:LYS:O	1:A:744:THR:HG22	2.08	0.54
1:B:88:ARG:HG3	1:B:283:PRO:HB2	1.88	0.54
1:B:677:ILE:O	1:B:920:ILE:HG21	2.08	0.53
1:A:577:PHE:HA	7:A:1417:HOH:O	2.08	0.53
1:B:351:GLU:HG3	1:B:395:PHE:CE2	2.43	0.53
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.44	0.53
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.89	0.53
1:A:1061:ALA:O	1:A:1062:ALA:CB	2.55	0.53
1:A:259:MET:HE2	1:A:259:MET:HA	1.91	0.53
1:B:725:ALA:CB	1:B:731:ALA:HB2	2.39	0.53
1:A:779:GLY:O	1:A:783:LYS:HG3	2.08	0.53
1:A:444:LEU:HG	1:A:553:PRO:HB2	1.90	0.53
1:A:783:LYS:O	1:A:787:GLU:HG2	2.09	0.53
1:B:701:MET:HE1	1:B:720:MET:CE	2.30	0.53
1:B:1048:LYS:HD2	1:B:1098:ARG:NH2	2.23	0.53
1:A:195:GLU:OE2	1:A:385:ARG:HD2	2.09	0.53
1:B:393:GLN:HG3	1:B:431:TYR:HD2	1.74	0.52
1:B:62:LEU:CD1	1:B:93:MET:HE3	2.40	0.52
1:B:886:GLU:O	2:D:8:DA:H4'	2.09	0.52
1:A:402:ARG:HA	1:A:408:ILE:CG2	2.39	0.52
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.10	0.52
1:A:842:LYS:NZ	7:A:1729:HOH:O	2.43	0.52
1:B:999:LEU:HB2	1:B:1004:LEU:CD2	2.40	0.52
1:B:402:ARG:HA	1:B:408:ILE:CG2	2.39	0.51
1:A:306:GLY:CA	1:A:412:PRO:HG2	2.35	0.51
1:A:984:TYR:CE1	1:A:1037:ARG:HB2	2.46	0.51
1:B:66:ALA:O	1:B:70:LEU:HG	2.11	0.51
1:B:805:VAL:HB	1:B:809:LEU:HD23	1.92	0.51
1:A:228:LEU:HD23	1:A:854:LEU:O	2.11	0.51
1:B:328:GLN:HB3	1:B:419:MET:HE3	1.93	0.51
1:B:897:THR:HG22	1:B:904:ARG:HG2	1.91	0.51
1:A:305:PHE:HE1	1:A:401:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:ASN:OD1	1:B:268:LYS:HB2	2.12	0.50
1:B:362:MET:HE1	1:B:528:SER:HA	1.92	0.50
1:A:305:PHE:CE1	1:A:401:VAL:HG22	2.47	0.50
1:B:972:TYR:HB2	1:B:1057:ILE:HD13	1.93	0.50
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.11	0.50
1:A:463:PHE:HA	1:A:957:LEU:HD13	1.94	0.50
1:A:1004:LEU:HD12	1:A:1025:ILE:HG13	1.93	0.50
1:A:188:LEU:HD21	1:A:783:LYS:HG2	1.93	0.50
1:B:259:MET:CE	1:B:262:ILE:HD12	2.41	0.50
1:A:630:TYR:O	1:A:637:GLN:NE2	2.38	0.50
1:B:1017:ARG:O	1:B:1018:GLU:C	2.54	0.50
1:A:886:GLU:O	2:C:8:DA:H4'	2.12	0.49
1:B:1018:GLU:CG	1:B:1019:ASN:H	2.12	0.49
1:A:8:LEU:HD23	7:A:1785:HOH:O	2.12	0.49
1:B:20:VAL:HG23	1:B:138:VAL:O	2.12	0.49
1:A:269:THR:O	2:C:11:DA:H5'	2.13	0.49
1:A:701:MET:HE1	1:A:720:MET:HE2	1.94	0.49
1:B:612:TYR:CD2	1:B:673:LEU:HD23	2.47	0.49
1:A:422:VAL:HG12	1:A:922:PHE:HA	1.95	0.49
1:A:1012:LEU:O	1:A:1017:ARG:NH1	2.46	0.49
1:A:368:ASN:O	1:A:370:GLU:N	2.46	0.49
1:B:671:ASN:HB3	1:B:672:PRO:HD3	1.95	0.49
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.95	0.48
1:B:1013:GLU:O	1:B:1014:TYR:C	2.56	0.48
1:B:149:GLU:O	1:B:153:GLN:HG3	2.13	0.48
1:A:141:ASP:HB2	1:A:146:LYS:HE3	1.94	0.48
1:B:612:TYR:HD1	1:B:666:ARG:HH12	1.58	0.48
1:A:501:MET:HE1	1:A:519:LEU:HG	1.96	0.48
1:B:269:THR:O	2:D:11:DA:H5'	2.14	0.48
1:A:579:PRO:HD2	7:A:1593:HOH:O	2.14	0.48
1:B:88:ARG:HD3	1:B:282:ASP:OD1	2.13	0.48
1:B:711:ASP:C	1:B:713:ASN:H	2.22	0.48
1:A:213:LYS:NZ	1:A:301:GLU:OE2	2.25	0.48
1:A:368:ASN:C	1:A:370:GLU:H	2.22	0.48
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.49	0.48
1:A:351:GLU:HG3	1:A:395:PHE:CZ	2.49	0.47
1:A:95:HIS:HA	1:B:248:GLU:O	2.14	0.47
1:B:1096:GLU:OE2	1:B:1099:LYS:HD2	2.13	0.47
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.96	0.47
1:A:286:SER:O	1:A:400:GLN:HB2	2.15	0.47
1:A:597:LYS:HE2	1:A:602:HIS:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:858:GLU:O	1:A:862:ILE:HG13	2.13	0.47
1:A:394:LEU:O	1:A:398:ILE:HG12	2.15	0.47
1:A:965:ARG:NH1	7:A:1806:HOH:O	2.23	0.47
1:B:438:LEU:C	1:B:438:LEU:HD23	2.39	0.47
1:B:911:ALA:HB1	1:B:912:PRO:HD2	1.97	0.47
1:B:37:SER:HB3	1:B:231:THR:HG22	1.96	0.46
1:B:88:ARG:HD2	1:B:283:PRO:CD	2.45	0.46
1:B:259:MET:HA	1:B:259:MET:HE2	1.98	0.46
1:A:194:VAL:HG13	1:A:195:GLU:N	2.30	0.46
1:B:811:TYR:CE2	1:B:1039:ILE:HD11	2.51	0.46
1:A:224:PRO:O	1:A:857:LYS:HB2	2.16	0.46
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.97	0.46
1:B:213:LYS:HB2	1:B:213:LYS:HE2	1.60	0.46
1:A:557:GLU:HA	1:A:953:MET:O	2.16	0.46
1:A:832:LYS:O	1:A:836:GLN:HG2	2.16	0.45
1:B:249:SER:O	1:B:250:THR:OG1	2.28	0.45
1:A:16:TYR:HB3	1:A:19:LEU:HG	1.98	0.45
1:A:616:THR:HG23	1:A:664:LEU:HB2	1.98	0.45
1:A:1002:GLU:O	1:A:1005:GLU:HG2	2.16	0.45
1:B:561:VAL:O	1:B:562:THR:C	2.59	0.45
1:A:210:LEU:HB3	1:A:239:ALA:HB1	1.99	0.45
1:A:782:LEU:HD23	1:A:782:LEU:HA	1.76	0.45
1:B:929:ASP:HA	1:B:932:MET:HE3	1.99	0.45
1:B:1072:LYS:HA	1:B:1072:LYS:HE2	1.97	0.45
1:B:942:ALA:HA	1:B:943:PRO:HD3	1.88	0.45
1:A:764:THR:HG21	1:A:780:GLU:HB3	1.99	0.45
1:B:620:MET:HE3	7:B:1809:HOH:O	2.16	0.45
1:B:229:GLY:O	1:B:233:GLY:HA3	2.17	0.45
1:A:323:ARG:HD2	7:A:1642:HOH:O	2.16	0.45
1:A:673:LEU:C	1:A:673:LEU:HD12	2.42	0.45
1:B:318:ARG:NH1	2:D:7:DA:OP2	2.47	0.45
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.45
1:B:228:LEU:HD12	1:B:232:LYS:HD2	1.98	0.45
1:B:1017:ARG:O	1:B:1019:ASN:N	2.50	0.45
1:A:673:LEU:HD12	1:A:673:LEU:O	2.17	0.44
1:A:1002:GLU:HA	1:A:1005:GLU:OE2	2.17	0.44
1:B:444:LEU:HG	1:B:553:PRO:HB2	1.98	0.44
1:B:729:ALA:HA	1:B:732:GLU:HB2	1.98	0.44
1:A:127:ASN:HA	1:A:132:GLY:O	2.17	0.44
1:A:673:LEU:HD13	1:A:801:ILE:HG23	2.00	0.44
1:A:677:ILE:O	1:A:920:ILE:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1099:LYS:HD3	1:B:1100:GLN:HG3	1.99	0.44
1:A:257:VAL:HG12	1:A:259:MET:CE	2.46	0.44
1:B:471:LEU:HG	1:B:495:LEU:HD11	1.98	0.44
1:A:103:LEU:HD11	1:A:242:ILE:HG12	2.00	0.44
1:A:505:PHE:CE2	1:A:536:MET:HE1	2.53	0.44
1:B:554:LEU:O	1:B:957:LEU:HG	2.17	0.44
1:A:1053:VAL:O	1:A:1071:GLY:HA3	2.18	0.44
1:B:1088:ASN:O	1:B:1092:ARG:HG3	2.18	0.44
1:B:443:ILE:C	1:B:444:LEU:HD22	2.43	0.44
1:A:444:LEU:N	1:A:444:LEU:HD22	2.33	0.44
1:B:842:LYS:HD2	1:B:842:LYS:HA	1.71	0.43
2:D:22:DC:O3'	7:D:105:HOH:O	2.13	0.43
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.47	0.43
1:B:882:ILE:HD13	1:B:919:GLY:HA2	2.00	0.43
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.51	0.43
1:B:940:LYS:O	1:B:940:LYS:HE2	2.19	0.43
1:A:27:ALA:HB3	1:A:31:LYS:HG2	1.99	0.43
1:A:349:PHE:CD1	1:A:502:MET:HE1	2.54	0.43
1:B:207:VAL:HG11	1:B:905:VAL:HG21	2.00	0.43
1:B:303:MET:HE2	1:B:303:MET:HB3	1.96	0.43
1:B:949:ILE:HG22	1:B:949:ILE:O	2.18	0.43
1:A:438:LEU:HD23	1:A:438:LEU:C	2.43	0.43
1:A:762:THR:CB	1:A:764:THR:HG22	2.46	0.43
1:B:710:LYS:O	1:B:710:LYS:HG2	2.19	0.43
1:A:170:THR:CG2	1:A:201:MET:HE3	2.48	0.43
1:B:65:ARG:O	1:B:69:GLU:HG3	2.17	0.43
1:A:1002:GLU:H	1:A:1002:GLU:CD	2.25	0.43
1:A:134:LEU:HD23	1:A:134:LEU:HA	1.89	0.43
1:A:634:MET:N	1:A:635:PRO:CD	2.82	0.43
1:A:737:ARG:O	1:A:738:PHE:C	2.62	0.43
1:A:306:GLY:HA2	1:A:412:PRO:CG	2.41	0.43
1:A:51:SER:OG	1:A:57:ASP:OD2	2.30	0.43
1:B:496:LYS:HB3	1:B:497:PRO:HD3	2.01	0.43
1:B:1061:ALA:O	1:B:1062:ALA:CB	2.66	0.42
1:A:598:THR:HG22	1:A:1066:PRO:HD3	2.01	0.42
1:A:162:TRP:CD1	1:A:166:ALA:HB2	2.54	0.42
1:A:575:GLY:O	1:A:1046:ARG:HD2	2.19	0.42
1:B:172:ILE:HD12	1:B:172:ILE:N	2.34	0.42
1:B:369:LYS:HE3	1:B:369:LYS:HB2	1.91	0.42
1:A:1053:VAL:CG1	1:A:1054:ASN:N	2.82	0.42
1:B:654:ILE:HD11	1:B:668:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:O	1:B:400:GLN:HB2	2.19	0.42
1:B:447:LYS:HE3	1:B:447:LYS:HB2	1.90	0.42
1:A:706:LYS:HB2	1:A:706:LYS:HE3	1.85	0.42
1:A:920:ILE:HB	1:A:921:PRO:HD3	2.01	0.42
1:A:1053:VAL:C	1:A:1071:GLY:HA3	2.45	0.42
1:B:367:LEU:HD22	1:B:372:LEU:HD21	2.02	0.42
1:B:432:ASN:HB2	1:B:433:PRO:HD2	2.01	0.42
1:B:972:TYR:OH	1:B:1051:ASP:OD1	2.31	0.42
1:B:669:ALA:C	1:B:672:PRO:HD2	2.45	0.42
1:B:671:ASN:HD21	1:B:688:LYS:HD2	1.84	0.42
1:A:89:TYR:O	1:A:93:MET:HG2	2.20	0.41
1:A:178:VAL:HG21	1:A:194:VAL:HA	2.02	0.41
1:A:355:LYS:O	1:A:359:LEU:HG	2.20	0.41
1:A:1095:LEU:O	1:A:1099:LYS:HG3	2.20	0.41
2:D:15:DG:H2''	2:D:16:DG:C8	2.55	0.41
1:A:254:GLU:OE1	1:A:273:TYR:OH	2.35	0.41
1:A:399:GLU:OE1	1:A:399:GLU:HA	2.21	0.41
1:A:814:GLU:O	1:A:818:LYS:HG3	2.20	0.41
1:A:831:PHE:O	1:A:835:VAL:HG23	2.21	0.41
1:B:802:THR:HG23	1:B:810:VAL:HG21	2.02	0.41
1:A:730:HIS:O	1:A:733:GLU:HG2	2.20	0.41
1:A:830:MET:O	1:A:834:ARG:HG2	2.20	0.41
1:B:135:LEU:O	1:B:138:VAL:HG22	2.20	0.41
2:D:3:DT:H2''	7:D:125:HOH:O	2.19	0.41
1:A:857:LYS:HD3	1:A:857:LYS:C	2.46	0.41
1:A:10:GLU:HA	1:A:13:ASP:HB3	2.03	0.41
1:B:228:LEU:O	1:B:232:LYS:HB2	2.21	0.41
1:B:724:GLN:HG2	7:B:1645:HOH:O	2.20	0.41
1:B:1004:LEU:HD13	1:B:1004:LEU:HA	1.84	0.41
1:A:213:LYS:HB2	1:A:213:LYS:HE2	1.82	0.41
1:A:318:ARG:HB2	1:A:421:ARG:HH12	1.86	0.41
1:A:355:LYS:HD2	1:A:388:GLU:HG3	2.01	0.41
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.96	0.41
1:A:714:ILE:HD11	1:A:718:MET:HB3	2.02	0.41
1:A:1014:TYR:HD2	1:A:1014:TYR:O	2.04	0.41
1:B:502:MET:CE	1:B:536:MET:HE2	2.51	0.40
1:A:623:LEU:HD12	1:A:623:LEU:HA	1.93	0.40
1:A:838:LYS:HD3	1:A:838:LYS:HA	1.88	0.40
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.57	0.40
1:A:460:PHE:O	1:A:464:GLN:HG3	2.21	0.40
1:B:88:ARG:HD2	1:B:283:PRO:CG	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:VAL:O	1:A:520:ASN:HB2	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:1439:HOH:O	7:B:1605:HOH:O[1_455]	2.17	0.03

## 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	1094/1118 (98%)	1055 (96%)	34 (3%)	5 (0%)	24	21
1	B	1093/1118 (98%)	1055 (96%)	33 (3%)	5 (0%)	24	21
All	All	2187/2236 (98%)	2110 (96%)	67 (3%)	10 (0%)	24	21

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1018	GLU
1	B	1018	GLU
1	B	1062	ALA
1	A	369	LYS
1	A	779	GLY
1	A	1017	ARG
1	A	1062	ALA
1	B	633	ASN
1	B	779	GLY
1	B	1017	ARG

### 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	917/935 (98%)	888 (97%)	29 (3%)	34	35
1	B	916/935 (98%)	889 (97%)	27 (3%)	37	40
All	All	1833/1870 (98%)	1777 (97%)	56 (3%)	35	37

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	75	GLU
1	A	204	THR
1	A	210	LEU
1	A	216	SER
1	A	260	SER
1	A	272	LEU
1	A	284	ILE
1	A	300	THR
1	A	405	SER
1	A	444	LEU
1	A	471	LEU
1	A	603	ARG
1	A	616	THR
1	A	634	MET
1	A	649	LEU
1	A	673	LEU
1	A	781	GLN
1	A	838	LYS
1	A	908	SER
1	A	951	ASP
1	A	1004	LEU
1	A	1031	LEU
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1059	GLN
1	A	1093	GLU
1	B	7	GLU
1	B	76	THR
1	B	84	GLU
1	B	88	ARG
1	B	105	SER
1	B	210	LEU
1	B	228	LEU
1	B	272	LEU
1	B	279	ASP
1	B	300	THR
1	B	372	LEU
1	B	406	GLU
1	B	444	LEU
1	B	471	LEU
1	B	472	ASP
1	B	649	LEU
1	B	668	ILE
1	B	744	THR
1	B	838	LYS
1	B	1004	LEU
1	B	1027	ASN
1	B	1031	LEU
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU
1	B	1055	LEU
1	B	1059	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	44	GLN
1	A	376	HIS
1	A	404	GLN
1	A	464	GLN
1	A	506	ASN
1	A	563	ASN
1	A	671	ASN
1	A	815	GLN
1	A	856	GLN

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Mol	Chain	Res	Type
1	A	863	GLN
1	A	893	GLN
1	A	1035	ASN
1	A	1059	GLN
1	B	44	GLN
1	B	122	GLN
1	B	464	GLN
1	B	506	ASN
1	B	613	GLN
1	B	617	ASN
1	B	671	ASN
1	B	863	GLN
1	B	878	GLN
1	B	976	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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
3	ATP	A	1201	4	32,33,33	1.40	6 (18%)	48,52,52	1.72	11 (22%)
5	PO4	A	1203	-	4,4,4	0.96	0	6,6,6	0.61	0
5	PO4	B	1201	-	4,4,4	0.88	0	6,6,6	0.62	0
6	5GP	C	101	-	26,26,26	1.00	2 (7%)	39,40,40	1.74	9 (23%)

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	ATP	A	1201	4	-	5/22/38/38	0/3/3/3
6	5GP	C	101	-	-	5/10/26/26	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ATP	C5-C4	4.52	1.47	1.39
3	A	1201	ATP	C5-C6	2.65	1.48	1.41
6	C	101	5GP	C6-N1	-2.55	1.34	1.38
3	A	1201	ATP	C5-N7	-2.35	1.34	1.39
3	A	1201	ATP	C8-N7	2.15	1.35	1.31
3	A	1201	ATP	C4-N9	-2.10	1.33	1.37
6	C	101	5GP	C5-N7	-2.03	1.35	1.39
3	A	1201	ATP	PB-O3A	2.03	1.61	1.59

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	5GP	C5-C4-N3	-5.50	119.64	128.39
3	A	1201	ATP	C5-C4-N3	-5.47	119.18	126.72
6	C	101	5GP	C2-N3-C4	4.49	120.04	112.30
3	A	1201	ATP	N3-C4-N9	4.38	134.62	127.17
3	A	1201	ATP	C2-N3-C4	3.56	120.53	111.83
3	A	1201	ATP	C4-C5-N7	-3.50	106.58	110.58
3	A	1201	ATP	N3-C2-N1	-3.28	123.62	128.58
6	C	101	5GP	N9-C4-N3	3.25	132.44	125.95
3	A	1201	ATP	C2'-C1'-N9	-2.96	105.96	113.30
3	A	1201	ATP	C4-N9-C8	2.94	108.83	105.74
6	C	101	5GP	OP2-P-O5'	-2.93	99.03	106.67
3	A	1201	ATP	C5-N7-C8	2.60	107.54	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	5GP	C5-C6-N1	2.38	119.31	113.25
6	C	101	5GP	N9-C8-N7	-2.38	109.00	113.40
6	C	101	5GP	O6-C6-C5	-2.25	120.60	126.53
6	C	101	5GP	C2-N1-C6	-2.23	121.06	125.11
3	A	1201	ATP	C6-C5-N7	2.22	136.38	132.09
3	A	1201	ATP	N9-C8-N7	-2.17	110.86	113.94
6	C	101	5GP	C4-C5-N7	-2.09	107.35	110.67
3	A	1201	ATP	C2-N1-C6	2.07	122.12	118.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	ATP	C5'-O5'-PA-O1A
3	A	1201	ATP	C5'-O5'-PA-O3A
6	C	101	5GP	C5'-O5'-P-OP1
6	C	101	5GP	C5'-O5'-P-OP3
6	C	101	5GP	C5'-O5'-P-OP2
6	C	101	5GP	C3'-C4'-C5'-O5'
6	C	101	5GP	O4'-C4'-C5'-O5'
3	A	1201	ATP	PB-O3B-PG-O1G
3	A	1201	ATP	PB-O3B-PG-O3G
3	A	1201	ATP	C5'-O5'-PA-O2A

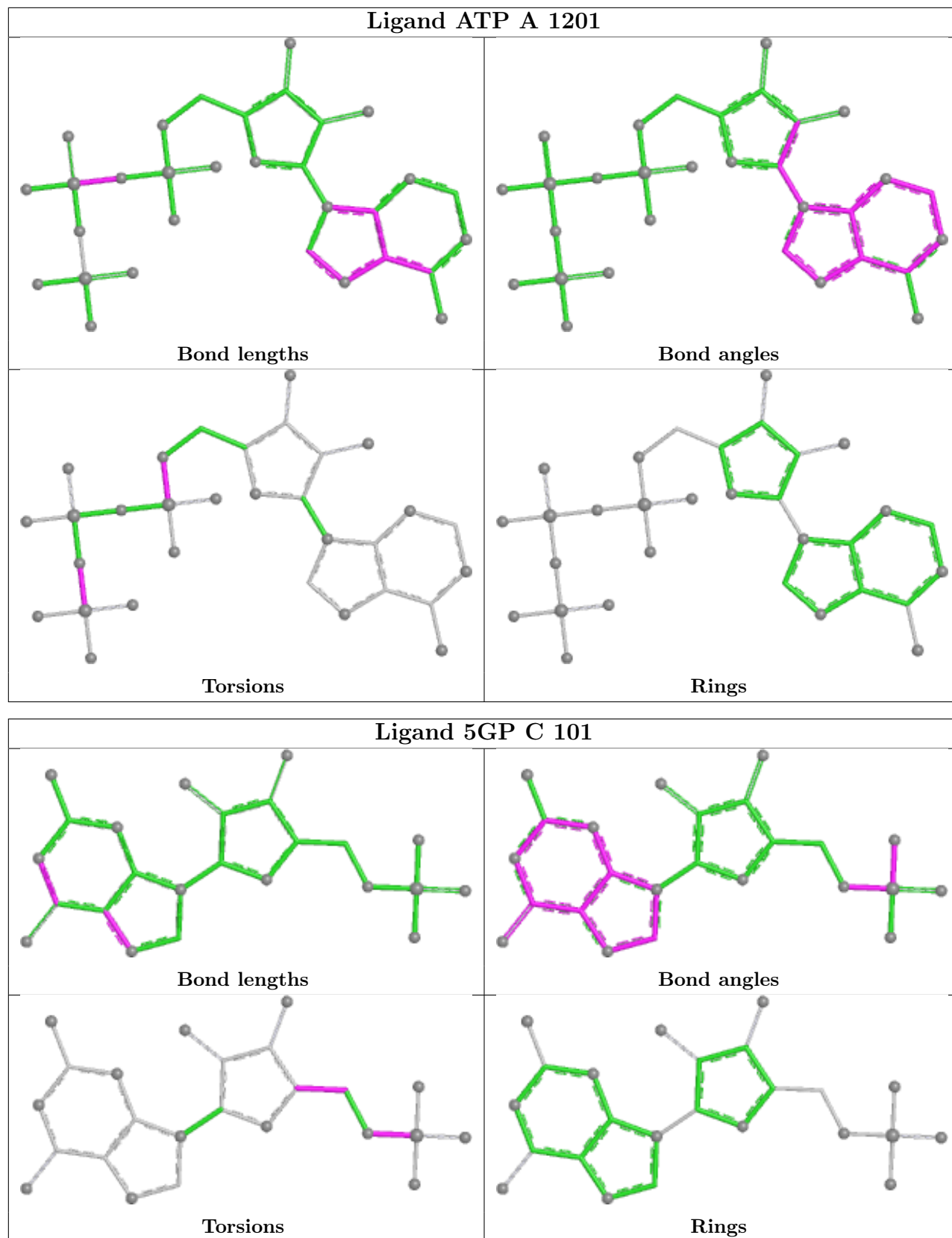
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1203	PO4	1	0
5	B	1201	PO4	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1095/1118 (97%)	0.09	50 (4%) 37 36	10, 28, 69, 101	1 (0%)
1	B	1095/1118 (97%)	0.14	69 (6%) 26 24	11, 27, 66, 130	0
2	C	20/36 (55%)	-0.12	0 100 100	26, 37, 61, 66	0
2	D	20/36 (55%)	-0.13	1 (5%) 34 33	22, 36, 61, 80	0
All	All	2230/2308 (96%)	0.11	120 (5%) 31 30	10, 28, 67, 130	1 (0%)

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1014	TYR	5.9
1	B	726	ALA	5.3
1	B	729	ALA	5.3
1	B	731	ALA	5.2
1	B	1099	LYS	4.3
1	B	730	HIS	4.1
1	B	1100	GLN	4.1
1	B	725	ALA	4.1
1	A	262	ILE	4.0
1	B	727	SER	4.0
1	B	766	ALA	3.8
1	B	262	ILE	3.7
1	A	661	ALA	3.7
1	B	714	ILE	3.6
1	B	765	GLY	3.6
1	A	729	ALA	3.5
1	B	712	PRO	3.5
1	A	1014	TYR	3.3
1	B	716	ALA	3.3
1	A	725	ALA	3.2
1	A	714	ILE	3.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	1019	ASN	3.1
1	B	281	PHE	3.1
1	B	709	ALA	3.1
1	B	678	TYR	3.0
1	A	1099	LYS	3.0
1	B	707	ALA	2.9
1	A	844	LYS	2.9
1	A	371	LEU	2.9
1	B	754	LYS	2.9
1	B	763	GLY	2.9
1	A	770	ILE	2.8
1	B	767	LYS	2.8
1	B	732	GLU	2.8
1	A	709	ALA	2.8
1	A	1097	ALA	2.8
1	B	708	ARG	2.7
1	A	910	TYR	2.7
1	A	659	ASN	2.7
1	B	723	LYS	2.7
1	A	843	ALA	2.7
1	B	654	ILE	2.7
1	B	188	LEU	2.7
1	B	770	ILE	2.6
1	B	728	GLU	2.6
1	B	962	ASP	2.6
1	B	677	ILE	2.6
1	A	658	GLU	2.6
1	B	28	GLU	2.6
1	A	281	PHE	2.6
1	B	525	ASP	2.6
1	B	1018	GLU	2.6
1	B	768	GLY	2.6
1	A	719	ALA	2.6
1	A	726	ALA	2.6
1	B	8	LEU	2.6
1	A	1005	GLU	2.5
1	B	91	GLU	2.5
1	A	1095	LEU	2.5
1	B	665	LYS	2.5
1	B	1034	ARG	2.5
1	A	258	ASP	2.5
1	A	657	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	457	ASN	2.5
1	B	431	TYR	2.5
1	B	1016	GLN	2.4
1	B	652	PRO	2.4
1	A	717	ALA	2.4
1	B	1098	ARG	2.4
1	A	730	HIS	2.4
1	B	371	LEU	2.4
1	B	6	GLU	2.4
1	B	191	GLU	2.4
1	A	767	LYS	2.3
1	B	764	THR	2.3
1	A	707	ALA	2.3
1	A	265	ASP	2.3
1	A	307	ASP	2.3
1	B	718	MET	2.3
1	B	769	LYS	2.3
1	B	621	GLU	2.3
1	B	27	ALA	2.3
1	A	191	GLU	2.3
1	A	710	LYS	2.3
1	A	731	ALA	2.3
1	B	187	ALA	2.2
1	A	431	TYR	2.2
1	B	710	LYS	2.2
1	A	766	ALA	2.2
1	A	1018	GLU	2.2
1	A	727	SER	2.2
1	B	658	GLU	2.2
1	B	910	TYR	2.2
1	A	712	PRO	2.1
1	A	6	GLU	2.1
1	B	10	GLU	2.1
1	A	8	LEU	2.1
1	B	721	PHE	2.1
1	A	183	GLY	2.1
1	B	666	ARG	2.1
2	D	3	DT	2.1
1	A	190	PRO	2.1
1	A	264	PRO	2.1
1	A	1100	GLN	2.1
1	B	752	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	70	LEU	2.1
1	A	43	GLU	2.1
1	B	807	GLU	2.1
1	B	653	ASP	2.1
1	B	753	ARG	2.1
1	B	722	GLY	2.1
1	A	260	SER	2.1
1	B	719	ALA	2.1
1	B	656	LEU	2.0
1	B	711	ASP	2.0
1	A	76	THR	2.0
1	A	716	ALA	2.0
1	A	708	ARG	2.0
1	A	754	LYS	2.0
1	B	706	LYS	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 oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

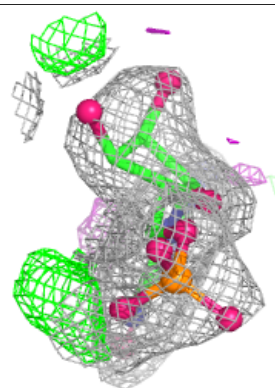
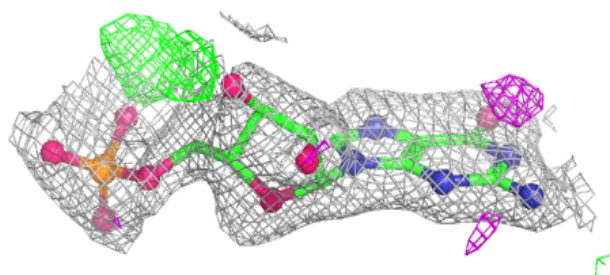
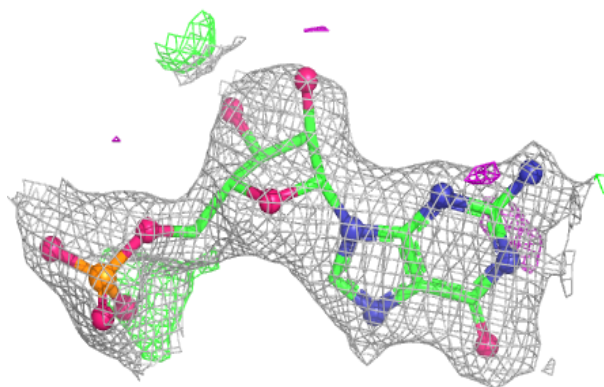
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	5GP	C	101	24/24	0.77	0.13	36,47,75,96	0
3	ATP	A	1201	31/31	0.90	0.13	27,41,62,234	0
5	PO4	B	1201	5/5	0.92	0.13	42,46,51,54	0
5	PO4	A	1203	5/5	0.95	0.11	39,41,43,49	0
4	MN	A	1202	1/1	0.96	0.10	55,55,55,55	0

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.

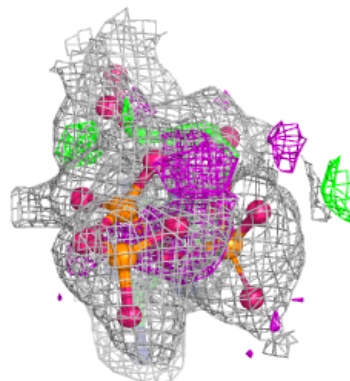
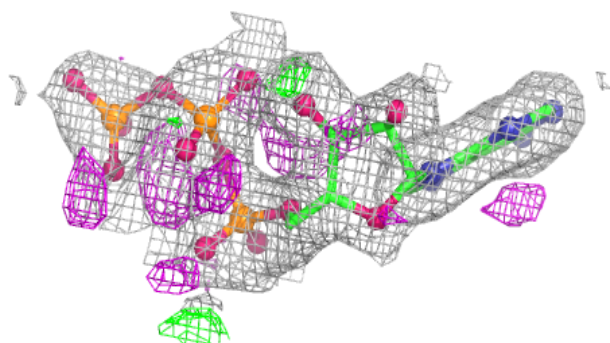
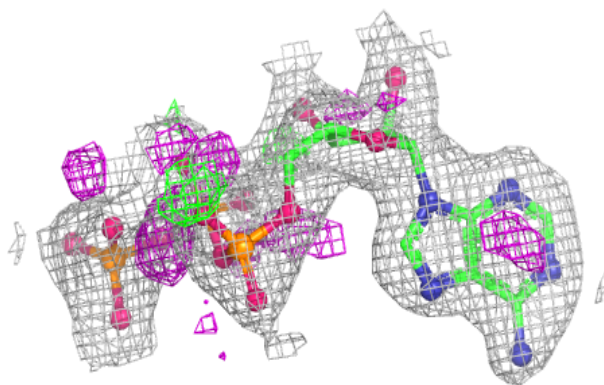
**Electron density around 5GP C 101:**

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



**Electron density around ATP A 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 [i](#)

There are no such residues in this entry.