



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 04:39 pm BST

PDB ID : 4FF2
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

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

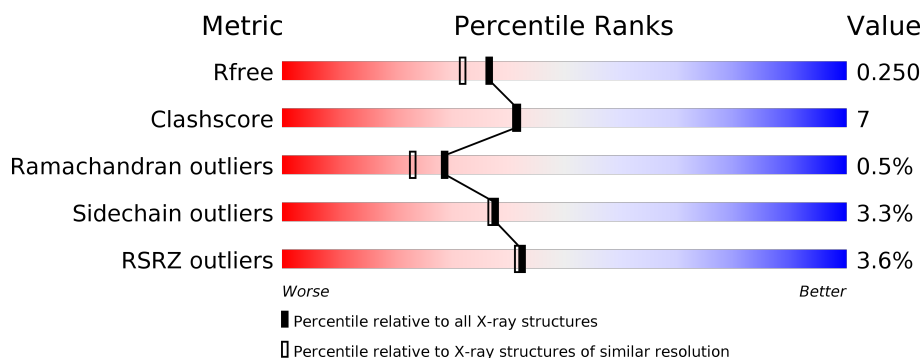
1 Overall quality at a glance

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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 $\leq 5\%$. 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	<div> <div>3%</div> <div> <div></div> <div>80%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	1118	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
2	C	36	<div> <div>47%</div> <div>8%</div> <div>44%</div> </div>
2	D	36	<div> <div>33%</div> <div>19%</div> <div>•</div> <div>44%</div> </div>

2 Entry composition

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
1	A	1095	Total	C	N	O	S	0	1	0
			8462	5310	1436	1675	41			
1	B	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			

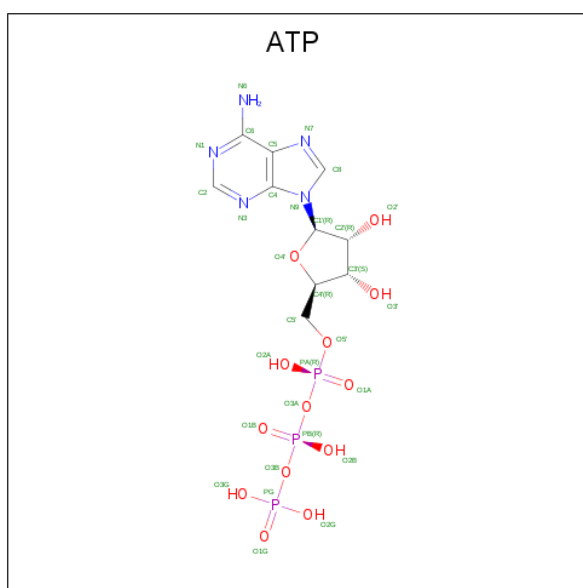
There are 24 discrepancies between the modelled and reference sequences:

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-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

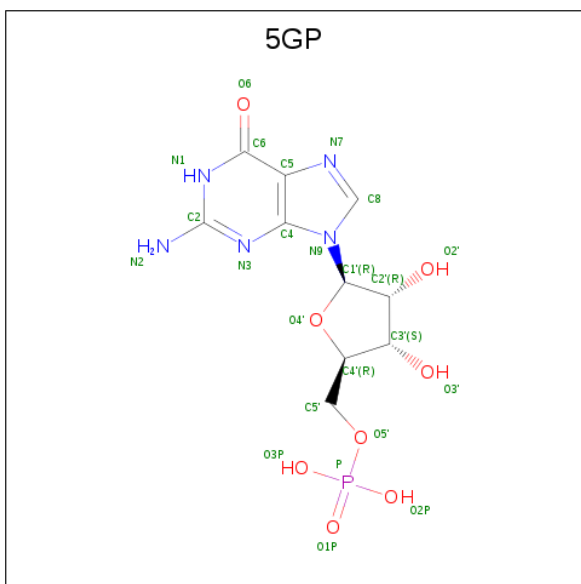
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mn	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

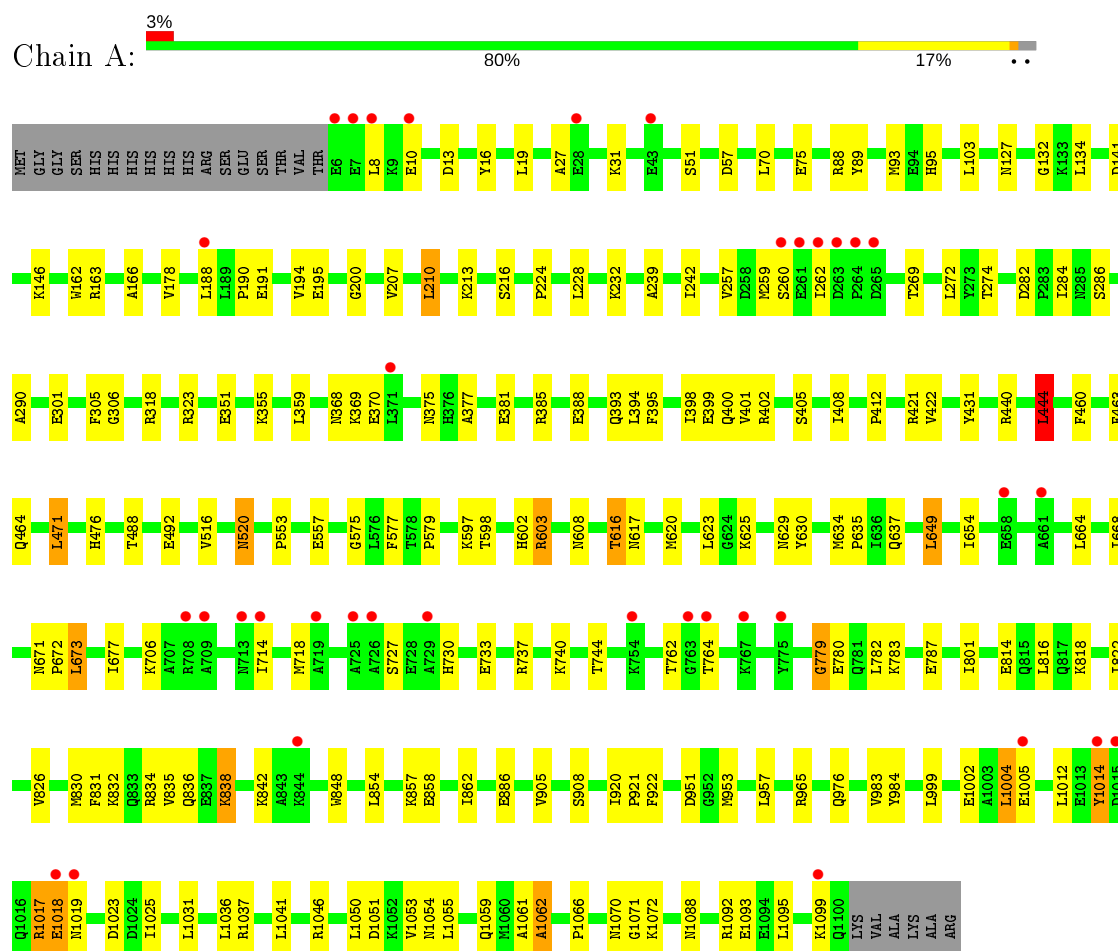
- Molecule 7 is water.

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

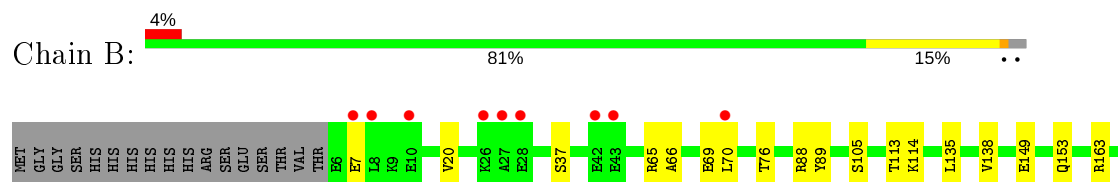
3 Residue-property plots [i](#)

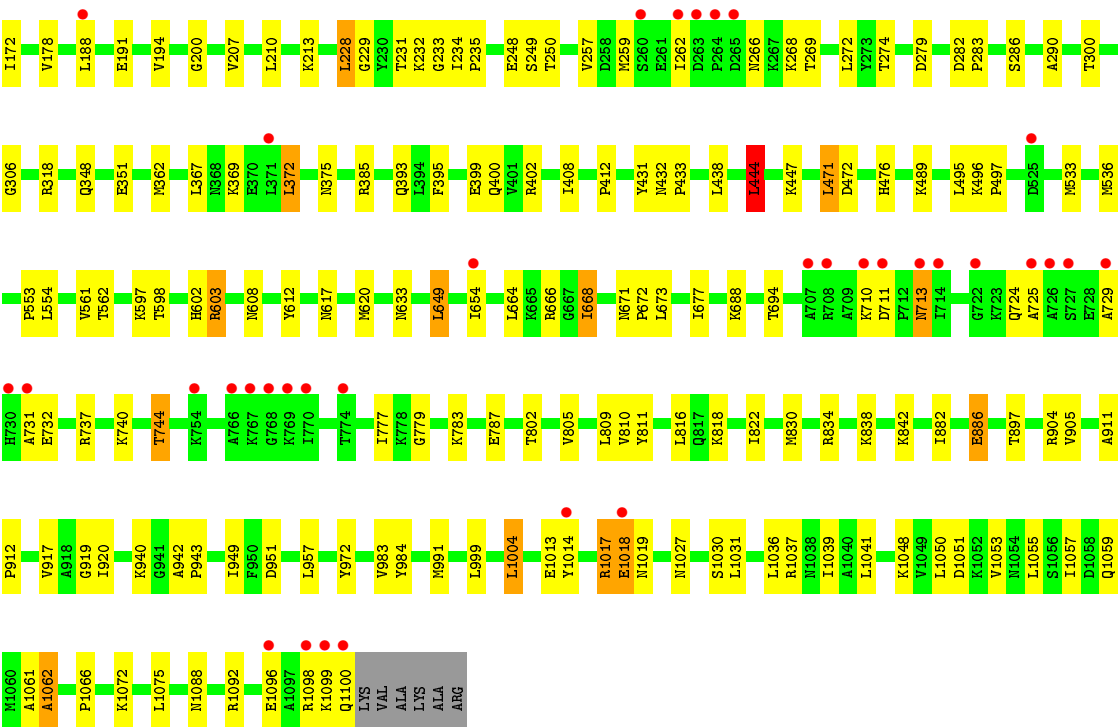
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

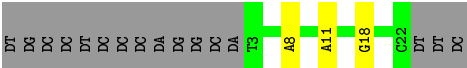


• Molecule 1: Virion RNA polymerase

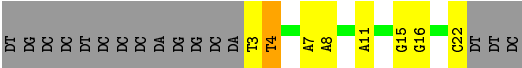
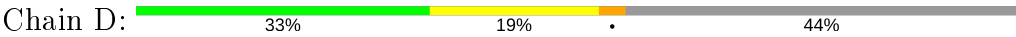




● Molecule 2: Bacteriophage N4 P2 promoter



● Molecule 2: Bacteriophage N4 P2 promoter



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.91Å 111.44Å 275.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.00 47.67 – 1.99	Depositor EDS
% Data completeness (in resolution range)	90.7 (47.67-2.00) 86.0 (47.67-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 1.98Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.208 , 0.255 0.202 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.116	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	18981	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, 5GP, ATP, 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	0.27	0/8591	0.44	1/11620 (0.0%)
1	B	0.26	0/8583	0.45	1/11609 (0.0%)
2	C	0.48	0/464	1.13	1/714 (0.1%)
2	D	0.51	0/464	1.12	1/714 (0.1%)
All	All	0.28	0/18102	0.51	4/24657 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	DT	O4'-C4'-C3'	-6.39	101.94	104.50
1	A	444	LEU	CA-CB-CG	6.01	129.11	115.30
2	C	18	DG	O4'-C1'-N9	5.95	112.16	108.00
1	B	444	LEU	CA-CB-CG	5.43	127.79	115.30

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	129	0
1	B	8454	0	8479	114	0
2	C	413	0	225	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	1
7	C	33	0	0	0	0
7	D	36	0	0	3	0
All	All	18981	0	17435	246	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 7.

All (246) 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: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:612:TYR:CE2	1:B:673:LEU:HD23	2.20	0.77
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:B:395:PHE:O	1:B:399:GLU:HG2	1.92	0.69
1:A:976:GLN:NE2	7:A:1339:HOH:O	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:1072:LYS:HE2	1.81	0.63
1:B:598:THR:HG22	1:B:1066:PRO:HD3	1.80	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: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
1:B:234:ILE:HB	1:B:235:PRO:HD3	1.87	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1061:ALA:O	1:A:1062:ALA:CB	2.55	0.53
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.89	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: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: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:984:TYR:CE1	1:A:1037:ARG:HB2	2.46	0.51
1:A:306:GLY:CA	1:A:412:PRO:HG2	2.35	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: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
1:B:266:ASN:OD1	1:B:268:LYS:HB2	2.12	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:A:718:MET:HE1	1:A:727:SER:O	2.11	0.49
1:B:1018:GLU:CG	1:B:1019:ASN:H	2.12	0.49
1:A:886:GLU:O	2:C:8:DA:H4'	2.12	0.49
1:A:8:LEU:HD23	7:A:1785:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:612:TYR:CD2	1:B:673:LEU:HD23	2.47	0.49
1:A:1012:LEU:O	1:A:1017:ARG:NH1	2.46	0.49
1:A:422:VAL:HG12	1:A:922:PHE:HA	1.95	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: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:A:259:MET:HE2	1:A:259:MET:HA	1.95	0.48
1:B:612:TYR:HD1	1:B:666:ARG:HH12	1.58	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
2:D:22:DC:O3'	7:D:105:HOH:O	2.13	0.48
1:A:213:LYS:NZ	1:A:301:GLU:OE2	2.25	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
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: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:617:ASN:HA	1:B:620:MET:HE2	1.96	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:1017:ARG:O	1:B:1018:GLU:C	2.54	0.46
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.97	0.46
1:B:213:LYS:HE2	1:B:213:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:TYR:HB3	1:A:19:LEU:HG	1.98	0.45
1:A:1002:GLU:O	1:A:1005:GLU:HG2	2.16	0.45
1:A:616:THR:HG23	1:A:664:LEU:HB2	1.98	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:1072:LYS:HE2	1:B:1072:LYS:HA	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:991:MET:HE2	1:B:1030:SER:HB3	1.99	0.45
1:B:229:GLY:O	1:B:233:GLY:HA3	2.17	0.45
1:B:362:MET:HB3	1:B:362:MET:HE3	1.86	0.45
1:A:323:ARG:HD2	7:A:1642:HOH:O	2.16	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:1017:ARG:O	1:B:1019:ASN:N	2.50	0.45
1:B:228:LEU:HD12	1:B:232:LYS:HD2	1.98	0.45
1:A:1002:GLU:HA	1:A:1005:GLU:OE2	2.17	0.44
1:A:673:LEU:HD12	1:A:673:LEU:O	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
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: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:1013:GLU:O	1:B:1014:TYR:C	2.56	0.44
1:B:1088:ASN:O	1:B:1092:ARG:HG3	2.18	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
1:A:816:LEU:CD1	1:A:983:VAL:HG21	2.47	0.43
1:B:536:MET:HE2	1:B:536:MET:HB2	1.93	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:HE2	1:B:940:LYS:O	2.19	0.43
1:A:27:ALA:HB3	1:A:31:LYS:HG2	1.99	0.43
1:B:207:VAL:HG11	1:B:905:VAL:HG21	2.00	0.43
1:B:949:ILE:O	1:B:949:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:762:THR:CB	1:A:764:THR:HG22	2.46	0.43
1:B:710:LYS:HG2	1:B:710:LYS:O	2.19	0.43
1:B:711:ASP:C	1:B:713:ASN:H	2.22	0.43
1:A:368:ASN:C	1:A:370:GLU:H	2.22	0.43
1:B:65:ARG:O	1:B:69:GLU:HG3	2.17	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: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:B:438:LEU:C	1:B:438:LEU:HD23	2.39	0.42
1:A:575:GLY:O	1:A:1046:ARG:HD2	2.19	0.42
1:A:162:TRP:CD1	1:A:166:ALA:HB2	2.54	0.42
1:A:259:MET:HE2	1:A:262:ILE:HD12	2.00	0.42
1:B:172:ILE:N	1:B:172:ILE:HD12	2.34	0.42
1:B:369:LYS:HB2	1:B:369:LYS:HE3	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
1:B:286:SER:O	1:B:400:GLN:HB2	2.19	0.42
1:B:447:LYS:HB2	1:B:447:LYS:HE3	1.90	0.42
1:A:706:LYS:HE3	1:A:706:LYS:HB2	1.85	0.42
1:A:920:ILE:HB	1:A:921:PRO:HD3	2.01	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: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:1095:LEU:O	1:A:1099:LYS:HG3	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
2:D:15:DG:H2"	2:D:16:DG:C8	2.55	0.41
1:A:399:GLU:HA	1:A:399:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1004:LEU:HD13	1:B:1004:LEU:HA	1.84	0.41
1:B:724:GLN:HG2	7:B:1645:HOH:O	2.20	0.41
1:A:1014:TYR:O	1:A:1014:TYR:HD2	2.04	0.41
1:A:213:LYS:HB2	1:A:213:LYS:HE2	1.82	0.41
1:A:355:LYS:HD2	1:A:388:GLU:HG3	2.01	0.41
1:A:318:ARG:HB2	1:A:421:ARG:HH12	1.86	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:673:LEU:HD12	1:A:673:LEU:C	2.42	0.40
1:B:561:VAL:O	1:B:562:THR:C	2.59	0.40
1:A:623:LEU:HD12	1:A:623:LEU:HA	1.93	0.40
1:A:838:LYS:HA	1:A:838:LYS:HD3	1.88	0.40
1:A:460:PHE:O	1:A:464:GLN:HG3	2.21	0.40
1:A:89:TYR:CZ	1:A:290:ALA:HB3	2.57	0.40
1:B:88:ARG:HD2	1:B:283:PRO:CG	2.50	0.40
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

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	1094/1118 (98%)	1055 (96%)	34 (3%)	5 (0%)	29	23
1	B	1093/1118 (98%)	1055 (96%)	33 (3%)	5 (0%)	29	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2187/2236 (98%)	2110 (96%)	67 (3%)	10 (0%)	29	23

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 ⓘ

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%)	39	38
1	B	916/935 (98%)	884 (96%)	32 (4%)	36	35
All	All	1833/1870 (98%)	1772 (97%)	61 (3%)	38	37

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	75	GLU
1	A	163	ARG
1	A	210	LEU
1	A	216	SER
1	A	260	SER
1	A	272	LEU
1	A	284	ILE

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Mol	Chain	Res	Type
1	A	405	SER
1	A	444	LEU
1	A	471	LEU
1	A	520	ASN
1	A	603	ARG
1	A	616	THR
1	A	649	LEU
1	A	673	LEU
1	A	838	LYS
1	A	908	SER
1	A	951	ASP
1	A	1004	LEU
1	A	1014	TYR
1	A	1023	ASP
1	A	1031	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	B	7	GLU
1	B	76	THR
1	B	105	SER
1	B	163	ARG
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	385	ARG
1	B	444	LEU
1	B	471	LEU
1	B	472	ASP
1	B	489	LYS
1	B	533	MET
1	B	603	ARG
1	B	649	LEU
1	B	668	ILE
1	B	713	ASN
1	B	744	THR

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Mol	Chain	Res	Type
1	B	838	LYS
1	B	886	GLU
1	B	951	ASP
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

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

Mol	Chain	Res	Type
1	A	506	ASN
1	A	671	ASN
1	B	44	GLN
1	B	122	GLN
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 [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 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	26,33,33	0.93	1 (3%)	31,52,52	1.35	4 (12%)
5	PO4	B	1201	-	4,4,4	0.84	0	6,6,6	0.59	0
6	5GP	C	101	-	22,26,26	0.61	0	27,40,40	1.81	5 (18%)
5	PO4	A	1203	-	4,4,4	0.91	0	6,6,6	0.58	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	ATP	A	1201	4	-	5/18/38/38	0/3/3/3
6	5GP	C	101	-	-	5/6/26/26	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	ATP	C5-C4	2.35	1.47	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	101	5GP	N3-C2-N1	-4.73	120.91	127.22
6	C	101	5GP	C2-N3-C4	4.10	120.04	115.36
3	A	1201	ATP	N3-C2-N1	-3.23	123.62	128.68
6	C	101	5GP	C6-N1-C2	3.23	121.06	115.93
3	A	1201	ATP	PB-O3B-PG	-3.18	121.90	132.83
6	C	101	5GP	C5-C6-N1	-3.01	119.31	123.43
6	C	101	5GP	O3P-P-O5'	-2.90	99.03	106.73
3	A	1201	ATP	C4-C5-N7	-2.71	106.58	109.40
3	A	1201	ATP	PA-O3A-PB	-2.46	124.39	132.83

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
6	C	101	5GP	C5'-O5'-P-O1P
6	C	101	5GP	C5'-O5'-P-O2P
6	C	101	5GP	C5'-O5'-P-O3P
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-O3A
3	A	1201	ATP	C5'-O5'-PA-O2A

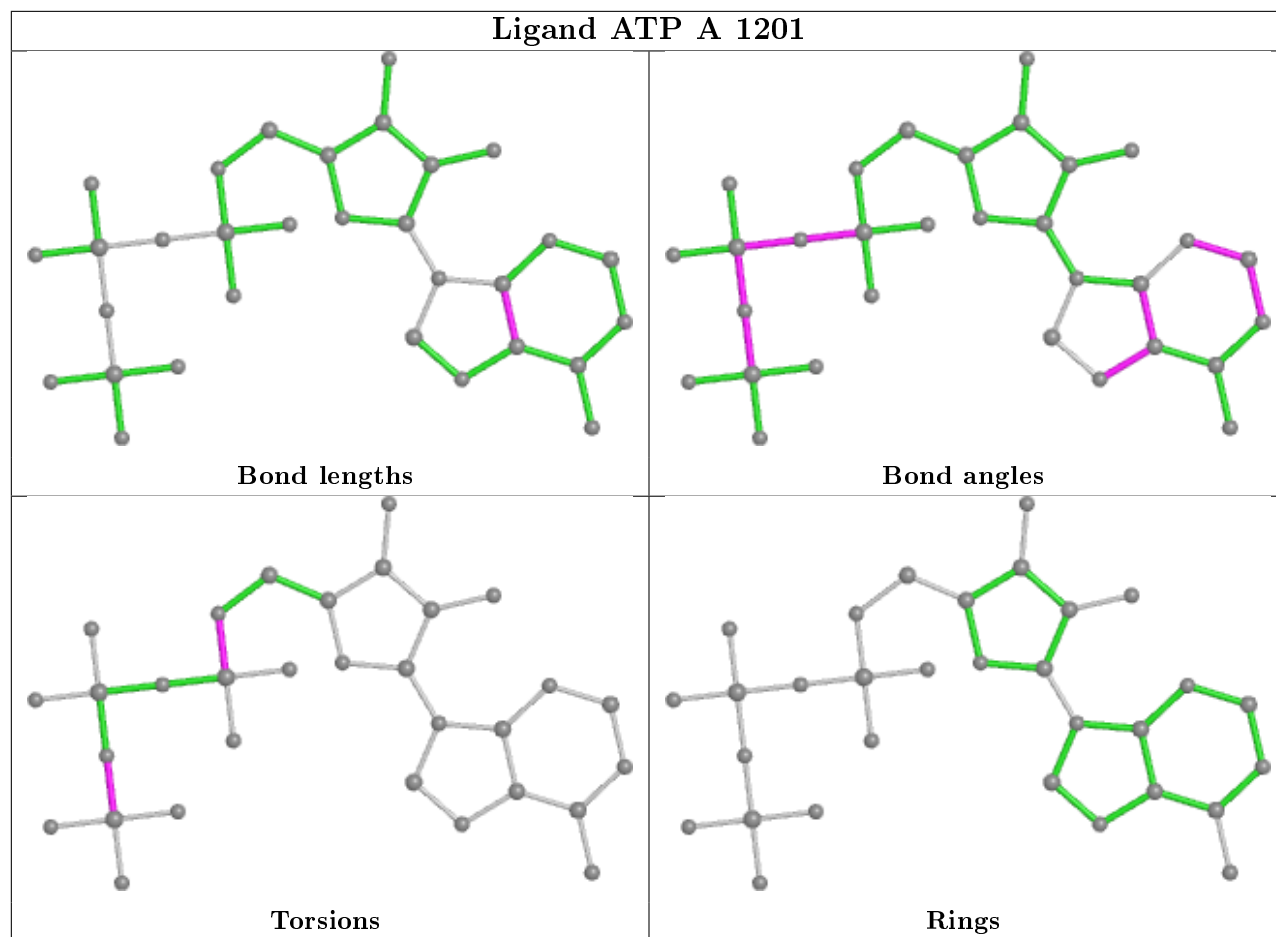
There are no ring outliers.

2 monomers are involved in 2 short contacts:

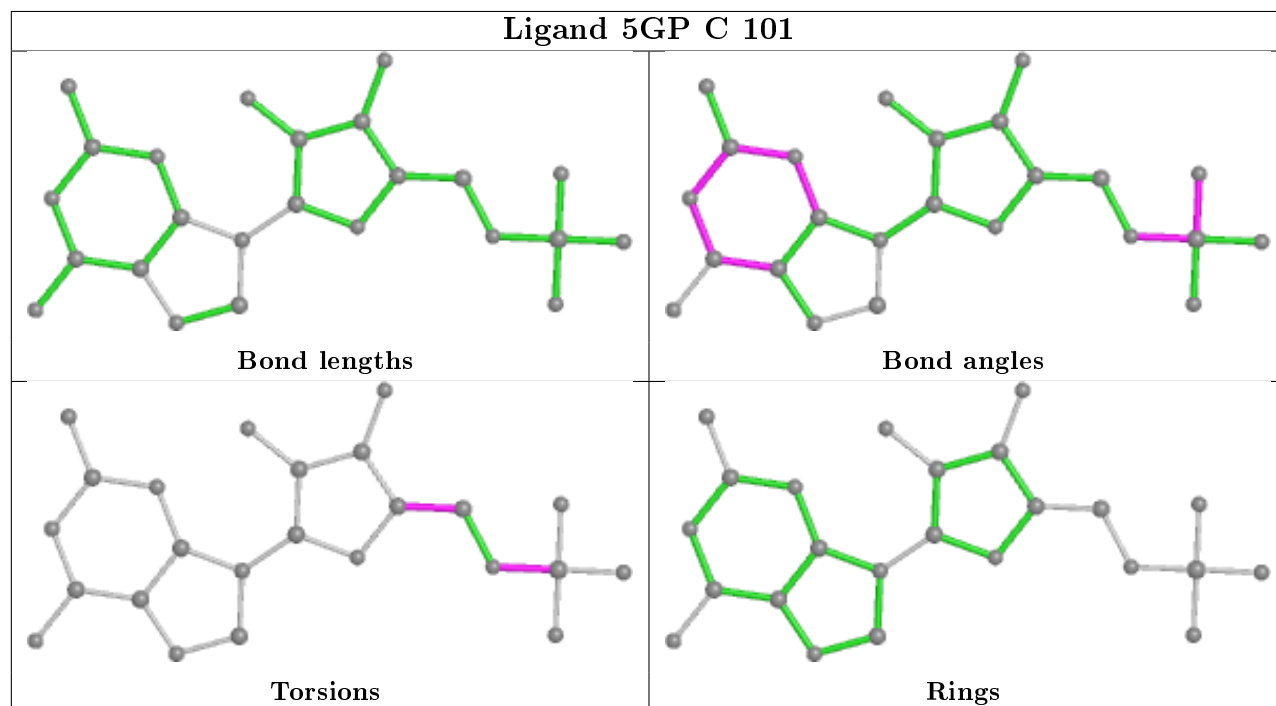
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1201	PO4	1	0
5	A	1203	PO4	1	0

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.

Ligand ATP A 1201



Ligand 5GP C 101



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(Å ²)	Q<0.9
1	A	1095/1118 (97%)	-0.02	36 (3%) 46 45	10, 28, 69, 101	0
1	B	1095/1118 (97%)	0.05	44 (4%) 38 37	11, 27, 66, 130	0
2	C	20/36 (55%)	-0.35	0 100 100	26, 37, 61, 66	0
2	D	20/36 (55%)	-0.36	0 100 100	22, 36, 61, 80	0
All	All	2230/2308 (96%)	0.01	80 (3%) 42 42	10, 28, 67, 130	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1014	TYR	7.6
1	B	726	ALA	7.5
1	B	1099	LYS	6.6
1	B	767	LYS	6.5
1	B	1100	GLN	6.3
1	B	713	ASN	5.9
1	B	1018	GLU	5.7
1	B	730	HIS	5.4
1	B	727	SER	5.1
1	A	8	LEU	4.2
1	B	722	GLY	4.1
1	A	658	GLU	4.1
1	B	264	PRO	4.1
1	B	770	ILE	4.0
1	B	725	ALA	3.8
1	B	768	GLY	3.8
1	B	711	ASP	3.8
1	A	264	PRO	3.8
1	B	754	LYS	3.8
1	A	262	ILE	3.7
1	B	769	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	8	LEU	3.7
1	A	1099	LYS	3.7
1	A	729	ALA	3.6
1	A	265	ASP	3.6
1	A	28	GLU	3.5
1	B	28	GLU	3.4
1	A	1014	TYR	3.4
1	B	714	ILE	3.3
1	A	261	GLU	3.3
1	B	708	ARG	3.2
1	B	188	LEU	3.2
1	B	42	GLU	3.1
1	B	265	ASP	3.1
1	A	1019	ASN	3.1
1	B	1098	ARG	3.1
1	A	725	ALA	3.1
1	A	1018	GLU	3.1
1	A	7	GLU	3.1
1	A	754	LYS	3.0
1	B	1096	GLU	3.0
1	A	767	LYS	2.9
1	A	6	GLU	2.9
1	A	713	ASN	2.9
1	A	719	ALA	2.9
1	B	7	GLU	2.9
1	A	726	ALA	2.8
1	B	263	ASP	2.8
1	A	260	SER	2.8
1	A	1015	ASP	2.8
1	A	708	ARG	2.7
1	A	371	LEU	2.7
1	B	27	ALA	2.7
1	B	766	ALA	2.6
1	B	371	LEU	2.5
1	A	661	ALA	2.5
1	B	729	ALA	2.5
1	B	707	ALA	2.5
1	B	26	LYS	2.5
1	B	10	GLU	2.5
1	A	714	ILE	2.4
1	B	731	ALA	2.4
1	A	709	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	710	LYS	2.4
1	A	10	GLU	2.3
1	A	764	THR	2.3
1	B	654	ILE	2.3
1	A	43	GLU	2.2
1	A	775	TYR	2.2
1	B	525	ASP	2.2
1	A	1005	GLU	2.1
1	B	262	ILE	2.1
1	B	260	SER	2.1
1	A	844	LYS	2.1
1	A	188	LEU	2.1
1	B	70	LEU	2.1
1	A	763	GLY	2.1
1	A	263	ASP	2.1
1	B	43	GLU	2.1
1	B	774	THR	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 carbohydrates in this entry.

6.4 Ligands ⓘ

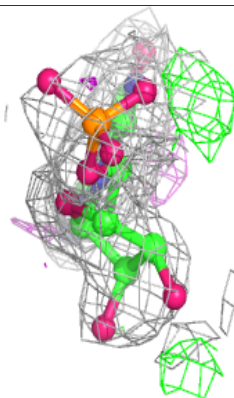
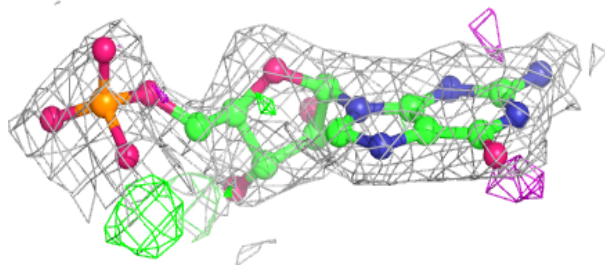
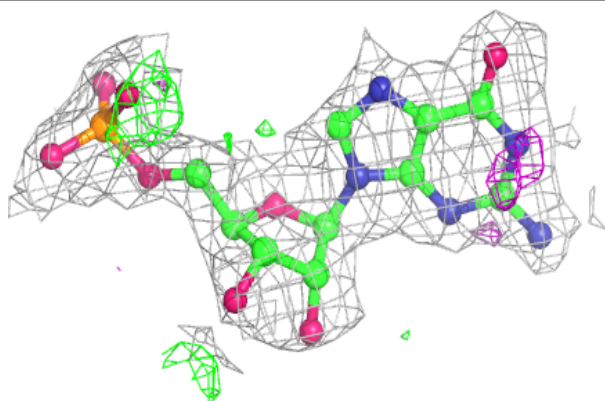
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	5GP	C	101	24/24	0.88	0.14	36,47,75,96	0
3	ATP	A	1201	31/31	0.91	0.15	27,41,62,234	0
4	MN	A	1202	1/1	0.93	0.06	55,55,55,55	0
5	PO4	B	1201	5/5	0.95	0.14	42,46,51,54	0
5	PO4	A	1203	5/5	0.97	0.12	39,41,43,49	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.

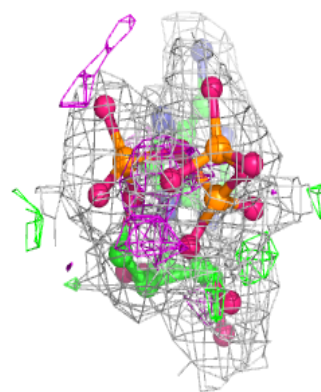
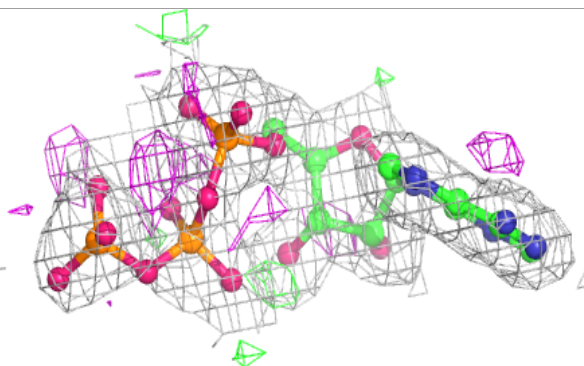
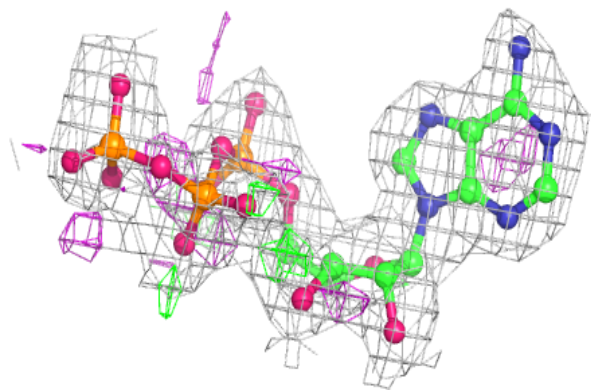
Electron density around 5GP C 101:

$2mF_o-DF_c$ (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.