



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:08 am BST

PDB ID : 4JKR
Title : Crystal Structure of E. coli RNA Polymerase in complex with ppGpp
Authors : Zuo, Y.; Wang, Y.; Steitz, T.A.
Deposited on : 2013-03-11
Resolution : 4.20 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

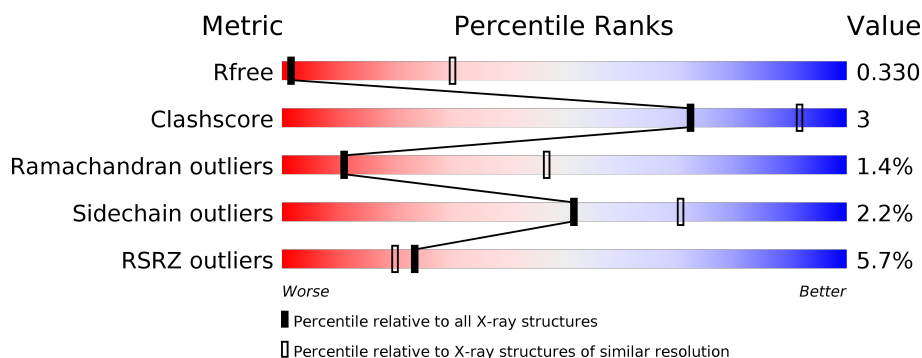
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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	329	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	
2	I	1342	

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Mol	Chain	Length	Quality of chain
3	D	1416	
3	J	1416	
4	E	90	
4	K	90	
5	F	628	
5	L	628	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58326 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	B	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	G	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			
1	H	227	Total	C	N	O	S	0	0	0
			1759	1096	311	346	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10569	6631	1841	2054	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10569	6631	1841	2054	43			

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1342	Total	C	N	O	S	0	0	0
			10431	6551	1860	1971	49			
3	J	1338	Total	C	N	O	S	0	0	0
			10401	6533	1854	1965	49			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1408	LEU	-	EXPRESSION TAG	UNP C5A0S8
D	1409	GLU	-	EXPRESSION TAG	UNP C5A0S8
D	1410	VAL	-	EXPRESSION TAG	UNP C5A0S8
D	1411	HIS	-	EXPRESSION TAG	UNP C5A0S8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1412	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1413	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1414	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1415	HIS	-	EXPRESSION TAG	UNP C5A0S8
D	1416	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1408	LEU	-	EXPRESSION TAG	UNP C5A0S8
J	1409	GLU	-	EXPRESSION TAG	UNP C5A0S8
J	1410	VAL	-	EXPRESSION TAG	UNP C5A0S8
J	1411	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1412	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1413	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1414	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1415	HIS	-	EXPRESSION TAG	UNP C5A0S8
J	1416	HIS	-	EXPRESSION TAG	UNP C5A0S8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	K	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			
5	L	481	Total	C	N	O	S	0	0	0
			3910	2445	699	743	23			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-14	MET	-	EXPRESSION TAG	UNP P00579
F	-13	ARG	-	EXPRESSION TAG	UNP P00579
F	-12	GLY	-	EXPRESSION TAG	UNP P00579
F	-11	SER	-	EXPRESSION TAG	UNP P00579
F	-10	HIS	-	EXPRESSION TAG	UNP P00579
F	-9	HIS	-	EXPRESSION TAG	UNP P00579
F	-8	HIS	-	EXPRESSION TAG	UNP P00579
F	-7	HIS	-	EXPRESSION TAG	UNP P00579

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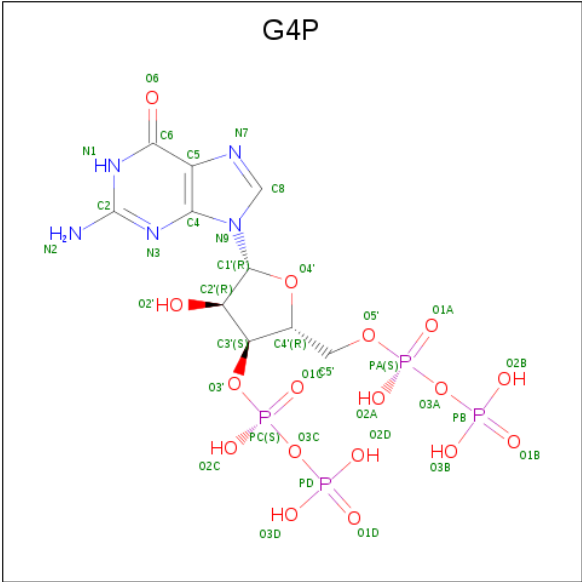
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Chain	Residue	Modelled	Actual	Comment	Reference
F	-6	HIS	-	EXPRESSION TAG	UNP P00579
F	-5	HIS	-	EXPRESSION TAG	UNP P00579
F	-4	THR	-	EXPRESSION TAG	UNP P00579
F	-3	ASP	-	EXPRESSION TAG	UNP P00579
F	-2	GLN	-	EXPRESSION TAG	UNP P00579
F	-1	PHE	-	EXPRESSION TAG	UNP P00579
F	0	THR	-	EXPRESSION TAG	UNP P00579
L	-14	MET	-	EXPRESSION TAG	UNP P00579
L	-13	ARG	-	EXPRESSION TAG	UNP P00579
L	-12	GLY	-	EXPRESSION TAG	UNP P00579
L	-11	SER	-	EXPRESSION TAG	UNP P00579
L	-10	HIS	-	EXPRESSION TAG	UNP P00579
L	-9	HIS	-	EXPRESSION TAG	UNP P00579
L	-8	HIS	-	EXPRESSION TAG	UNP P00579
L	-7	HIS	-	EXPRESSION TAG	UNP P00579
L	-6	HIS	-	EXPRESSION TAG	UNP P00579
L	-5	HIS	-	EXPRESSION TAG	UNP P00579
L	-4	THR	-	EXPRESSION TAG	UNP P00579
L	-3	ASP	-	EXPRESSION TAG	UNP P00579
L	-2	GLN	-	EXPRESSION TAG	UNP P00579
L	-1	PHE	-	EXPRESSION TAG	UNP P00579
L	0	THR	-	EXPRESSION TAG	UNP P00579

- Molecule 6 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	J	1	Total 1 Sr 1	0	0
6	D	1	Total 1 Sr 1	0	0
6	E	1	Total 1 Sr 1	0	0
6	I	1	Total 1 Sr 1	0	0
6	C	2	Total 2 Sr 2	0	0
6	A	1	Total 1 Sr 1	0	0
6	F	1	Total 1 Sr 1	0	0

- Molecule 7 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: C₁₀H₁₇N₅O₁₇P₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total	C	N	O	P	0	0
			36	10	5	17	4		
7	K	1	Total	C	N	O	P	0	0
			36	10	5	17	4		

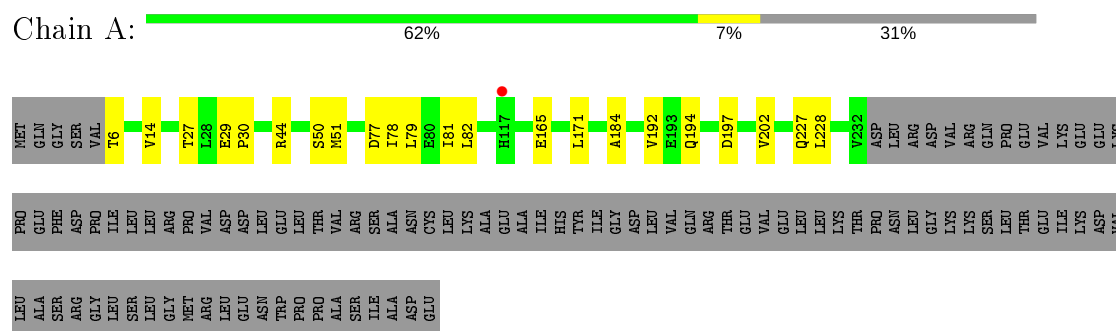
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

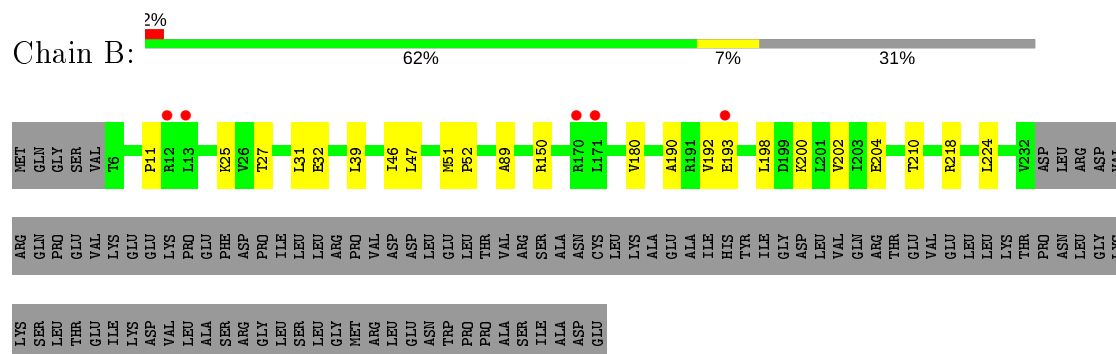
3 Residue-property plots [i](#)

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.

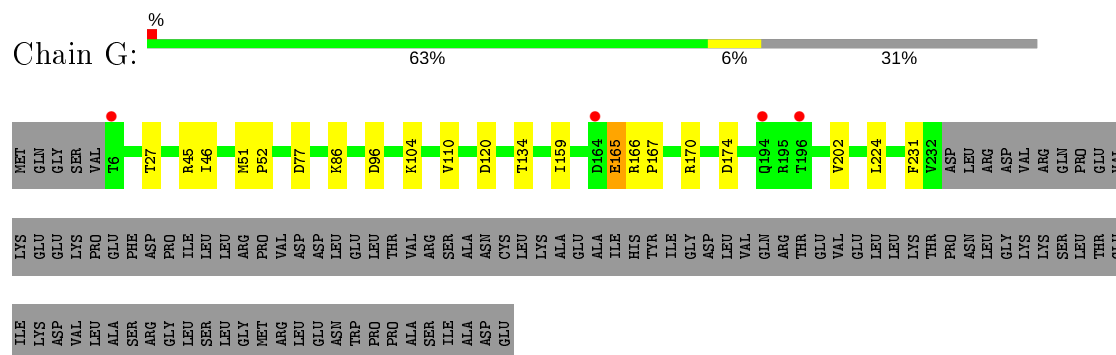
- Molecule 1: DNA-directed RNA polymerase subunit alpha



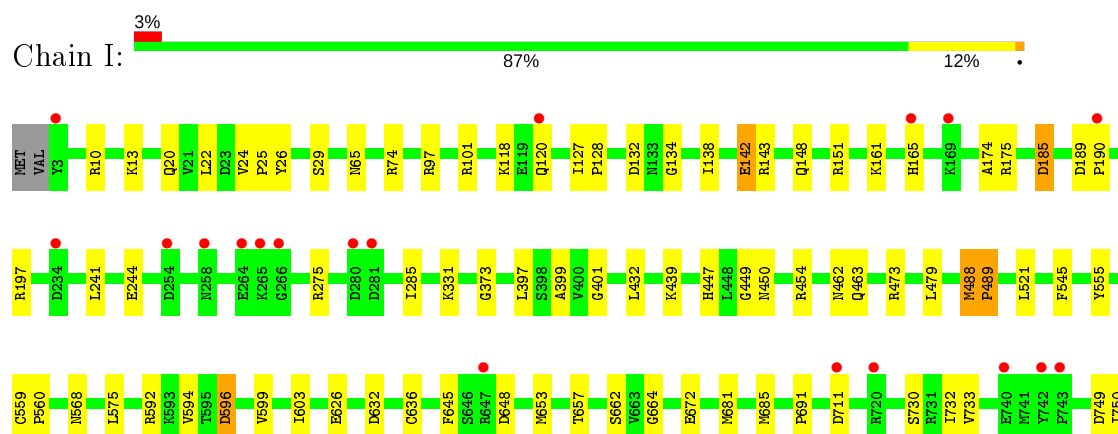
- Molecule 1: DNA-directed RNA polymerase subunit alpha

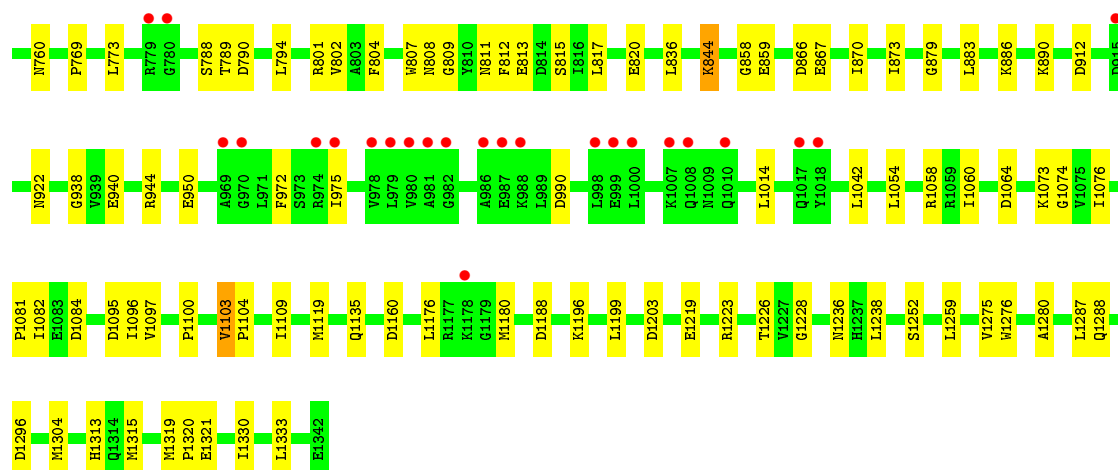


- Molecule 1: DNA-directed RNA polymerase subunit alpha




- Molecule 1: DNA-directed RNA polymerase subunit alpha

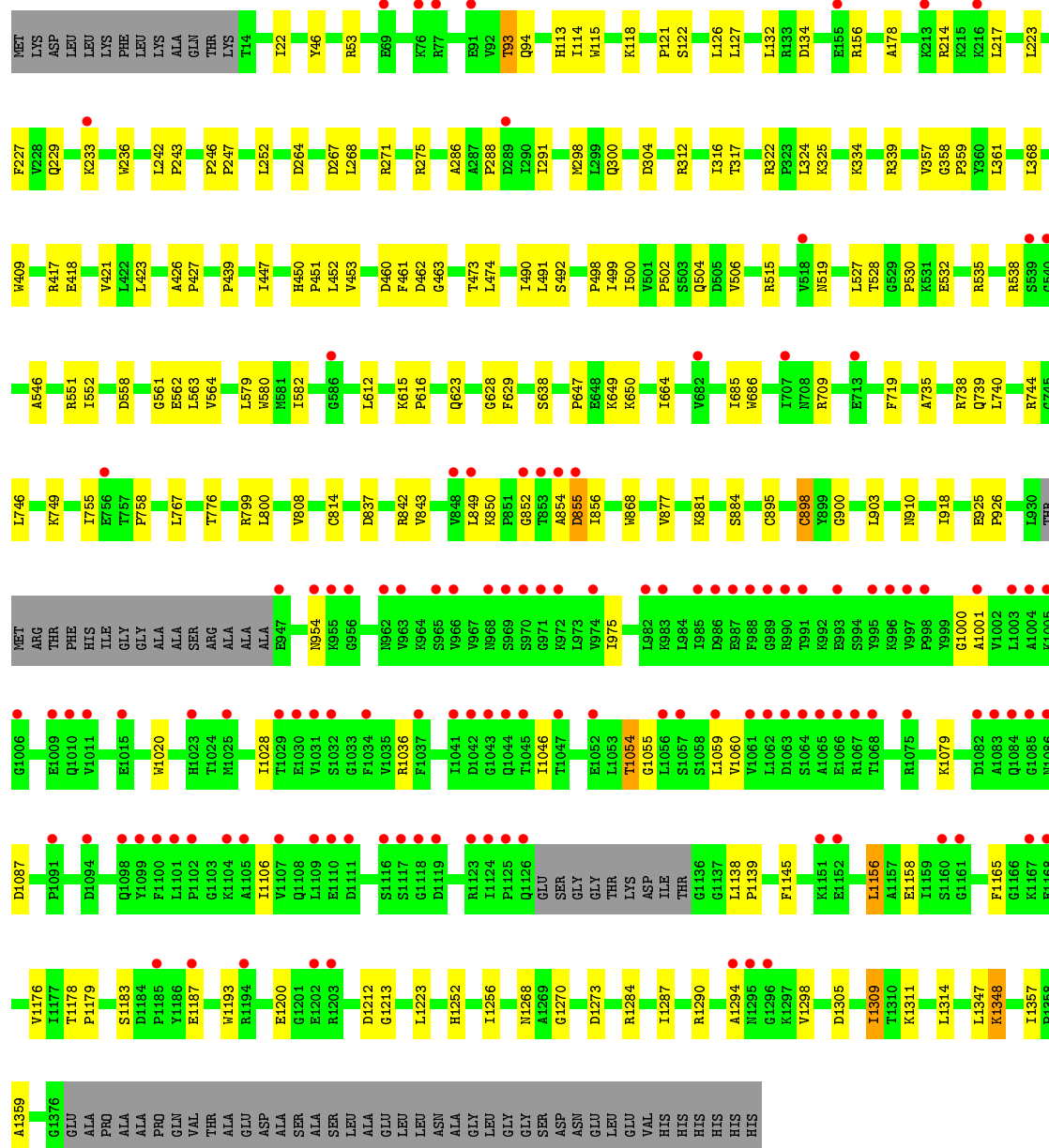





HIS
HIS
HIS

• Molecule 3: DNA-DIRECTED RNA POLYMERASE SUBUNIT BETA'

Chain J:  9% 80% 14% 6%

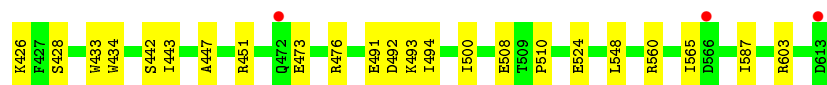
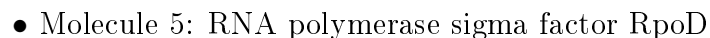
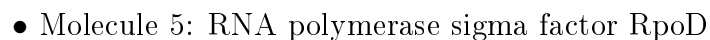


• Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  89% 11%



• Molecule 4: DNA-directed RNA polymerase subunit omega



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.57Å 206.16Å 311.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 4.20 39.94 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (39.97-4.20) 99.7 (39.94-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 4.13Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.247 , 0.318 0.260 , 0.330	Depositor DCC
R_{free} test set	4396 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	167.3	Xtriage
Anisotropy	0.268	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 202.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	58326	wwPDB-VP
Average B, all atoms (Å ²)	280.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.59% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, SR, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/1781	0.49	1/2414 (0.0%)
1	B	0.43	0/1781	0.51	1/2414 (0.0%)
1	G	0.41	0/1781	0.47	0/2414
1	H	0.40	0/1781	0.47	0/2414
2	C	0.50	0/10738	0.54	1/14489 (0.0%)
2	I	0.42	2/10738 (0.0%)	0.49	0/14489
3	D	0.50	5/10588 (0.0%)	0.53	2/14295 (0.0%)
3	J	0.45	7/10558 (0.1%)	0.51	1/14255 (0.0%)
4	E	0.53	0/710	0.56	0/956
4	K	0.39	0/710	0.51	0/956
5	F	0.45	3/3964 (0.1%)	0.52	0/5330
5	L	0.43	4/3964 (0.1%)	0.49	0/5330
All	All	0.46	21/59094 (0.0%)	0.51	6/79756 (0.0%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	479	GLU	CD-OE1	-6.85	1.18	1.25
2	I	807	TRP	CD2-CE2	5.79	1.48	1.41
3	D	580	TRP	CD2-CE2	5.54	1.48	1.41
3	D	33	TRP	CD2-CE2	5.48	1.48	1.41
3	J	868	TRP	CD2-CE2	5.42	1.47	1.41
3	J	686	TRP	CD2-CE2	5.40	1.47	1.41
3	J	580	TRP	CD2-CE2	5.39	1.47	1.41
3	J	1193	TRP	CD2-CE2	5.22	1.47	1.41
3	D	686	TRP	CD2-CE2	5.14	1.47	1.41
5	L	326	TRP	CD2-CE2	5.12	1.47	1.41
3	J	236	TRP	CD2-CE2	5.11	1.47	1.41
5	F	326	TRP	CD2-CE2	5.10	1.47	1.41
2	I	1276	TRP	CD2-CE2	5.08	1.47	1.41
3	D	1193	TRP	CD2-CE2	5.08	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	315	TRP	CD2-CE2	5.08	1.47	1.41
3	J	409	TRP	CD2-CE2	5.07	1.47	1.41
5	F	433	TRP	CD2-CE2	5.06	1.47	1.41
5	F	434	TRP	CD2-CE2	5.05	1.47	1.41
5	L	434	TRP	CD2-CE2	5.04	1.47	1.41
5	L	433	TRP	CD2-CE2	5.03	1.47	1.41
3	J	1020	TRP	CD2-CE2	5.00	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	218	ARG	NE-CZ-NH2	-6.97	116.81	120.30
2	C	1341	ASP	CB-CG-OD1	6.31	123.98	118.30
3	D	479	GLU	OE1-CD-OE2	-6.14	115.94	123.30
3	D	855	ASP	CB-CG-OD2	5.23	123.00	118.30
3	J	855	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	44	ARG	NE-CZ-NH2	-5.17	117.71	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1785	10	0
1	B	1759	0	1785	14	0
1	G	1759	0	1785	11	0
1	H	1759	0	1785	5	0
2	C	10569	0	10582	75	0
2	I	10569	0	10582	77	0
3	D	10431	0	10649	104	0
3	J	10401	0	10616	103	0
4	E	708	0	719	5	0
4	K	708	0	719	3	0
5	F	3910	0	3970	23	0
5	L	3910	0	3970	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	1	0	0	0	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
7	D	36	0	11	1	0
7	K	36	0	11	0	0
8	D	2	0	0	1	0
8	J	2	0	0	0	0
All	All	58326	0	58969	404	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 3.

All (404) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:895:CYS:HB2	3:J:898:CYS:SG	1.76	1.24
3:D:888:CYS:SG	3:D:895:CYS:SG	2.60	0.99
3:J:895:CYS:CB	3:J:898:CYS:SG	2.53	0.97
3:J:895:CYS:N	3:J:898:CYS:SG	2.42	0.93
3:D:898:CYS:O	3:D:898:CYS:SG	2.29	0.90
2:C:488:MET:HB2	2:C:489:PRO:HD3	1.55	0.88
3:J:814:CYS:SG	3:J:895:CYS:SG	2.74	0.85
3:D:855:ASP:OD1	3:D:856:ILE:N	2.12	0.82
2:C:560:PRO:HB2	3:D:776:THR:HG21	1.62	0.80
3:J:855:ASP:OD1	3:J:856:ILE:N	2.15	0.80
7:D:2001:G4P:C8	4:E:4:VAL:HG21	2.14	0.78
3:J:895:CYS:CA	3:J:898:CYS:SG	2.73	0.77
3:D:814:CYS:HB3	3:D:895:CYS:CB	2.15	0.76
3:D:888:CYS:SG	8:D:2003:ZN:ZN	1.75	0.75
3:D:325:LYS:HG3	5:F:508:GLU:HG3	1.70	0.74
1:A:14:VAL:HG21	1:A:29:GLU:HG2	1.70	0.72
2:I:1073:LYS:HD2	3:J:462:ASP:HB2	1.73	0.71
3:D:814:CYS:HB3	3:D:895:CYS:HB3	1.73	0.69
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.74	0.69
2:I:185:ASP:HB2	2:I:197:ARG:HB2	1.76	0.68
3:D:1145:PHE:HB3	3:D:1309:ILE:HD11	1.78	0.66
3:J:814:CYS:SG	3:J:895:CYS:HB2	2.35	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:241:LEU:HD11	2:I:285:ILE:HG12	1.76	0.66
2:C:870:ILE:HG12	2:C:944:ARG:HG2	1.78	0.65
2:C:1237:HIS:HB2	2:C:1242:LYS:HE2	1.78	0.65
2:I:447:HIS:HD2	2:I:449:GLY:H	1.46	0.64
2:C:1226:THR:HG22	3:D:638:SER:HB2	1.80	0.63
3:D:322:ARG:HH21	5:F:510:PRO:HG2	1.63	0.63
3:J:275:ARG:HE	3:J:298:MET:HB3	1.65	0.62
3:D:113:HIS:HD2	3:D:115:TRP:H	1.48	0.62
3:D:820:ILE:HA	3:D:1227:HIS:HE1	1.65	0.61
2:I:1103:VAL:H	2:I:1104:PRO:HD2	1.65	0.60
3:J:113:HIS:HD2	3:J:115:TRP:H	1.49	0.60
2:I:1226:THR:HG22	3:J:638:SER:HB2	1.83	0.60
3:D:849:LEU:O	3:D:851:PRO:HD3	2.01	0.59
2:C:447:HIS:HD2	2:C:449:GLY:H	1.49	0.59
2:C:870:ILE:HG21	2:C:1050:VAL:HG11	1.83	0.59
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.67	0.59
3:D:582:ILE:HG23	3:D:623:GLN:HB3	1.85	0.59
3:D:1054:THR:HG23	3:D:1055:GLY:HA2	1.85	0.59
2:C:563:THR:HG21	3:D:780:ARG:HD2	1.84	0.59
3:D:841:GLY:HA2	3:D:901:ARG:HD3	1.85	0.58
3:D:800:LEU:HD22	3:D:1256:ILE:HD13	1.85	0.58
2:C:488:MET:CB	2:C:489:PRO:HD3	2.30	0.58
2:I:1064:ASP:HB2	2:I:1076:ILE:HD12	1.85	0.58
3:J:1054:THR:HG23	3:J:1055:GLY:HA2	1.85	0.58
3:J:417:ARG:HG2	3:J:418:GLU:HG2	1.85	0.58
2:I:809:GLY:HA3	3:J:359:PRO:HB3	1.87	0.57
3:D:380:PHE:HB3	3:D:415:VAL:HG11	1.85	0.57
2:I:802:VAL:HG22	2:I:1096:ILE:HD11	1.86	0.57
3:D:814:CYS:HB3	3:D:895:CYS:SG	2.44	0.57
2:C:185:ASP:HB2	2:C:197:ARG:HB2	1.86	0.56
3:J:502:PRO:HB3	3:J:506:VAL:HB	1.88	0.56
3:J:271:ARG:O	3:J:275:ARG:HG2	2.05	0.56
5:F:284:GLU:HG3	5:F:344:LEU:HD11	1.86	0.56
2:C:1151:LEU:HD11	2:C:1201:LEU:HD22	1.87	0.56
2:I:820:GLU:HB2	2:I:1081:PRO:HA	1.88	0.56
5:L:242:HIS:H	5:L:245:ALA:HB3	1.71	0.56
3:D:968:ASN:HD21	3:D:972:LYS:HB2	1.71	0.55
3:J:368:LEU:HD12	3:J:439:PRO:HB3	1.87	0.55
3:J:800:LEU:HD22	3:J:1256:ILE:HD13	1.87	0.55
1:A:6:THR:HG23	1:B:150:ARG:HD3	1.88	0.55
2:I:488:MET:H	2:I:489:PRO:CD	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:801:ARG:HB2	2:C:1095:ASP:H	1.71	0.55
2:C:153:PRO:HD2	2:C:452:ARG:HD3	1.88	0.55
3:J:842:ARG:HH22	3:J:884:SER:HA	1.71	0.55
3:J:582:ILE:HG23	3:J:623:GLN:HB3	1.88	0.55
3:J:519:ASN:HB3	3:J:709:ARG:HB2	1.89	0.55
2:I:1176:LEU:HD22	2:I:1180:MET:HG2	1.88	0.54
3:D:905:ARG:HE	4:E:16:ARG:HH11	1.55	0.54
2:I:801:ARG:HB2	2:I:1095:ASP:H	1.73	0.54
3:D:890:THR:O	3:D:890:THR:HG22	2.06	0.54
4:E:38:LEU:HD11	4:E:67:ARG:HH12	1.73	0.54
3:J:735:ALA:HA	3:J:738:ARG:HD3	1.90	0.54
5:L:560:ARG:HG2	5:L:565:ILE:HB	1.90	0.54
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.90	0.53
2:I:521:LEU:HD11	2:I:664:GLY:HA2	1.90	0.53
3:D:1138:LEU:N	3:D:1139:PRO:HD2	2.24	0.53
3:D:1263:LYS:HE3	3:D:1315:ALA:HB1	1.91	0.53
3:J:368:LEU:HD11	3:J:421:VAL:HG11	1.91	0.53
3:J:850:LYS:HG3	3:J:877:VAL:HG13	1.91	0.53
2:I:867:GLU:HG3	2:I:944:ARG:HH11	1.74	0.53
3:J:615:LYS:HA	4:K:5:THR:HG21	1.91	0.53
1:B:32:GLU:HA	1:B:198:LEU:HD22	1.92	0.52
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	1.92	0.52
3:D:259:ARG:HD3	5:F:505:ILE:HD11	1.92	0.52
3:D:746:LEU:HG	3:D:758:PRO:HB3	1.91	0.52
2:I:812:PHE:HB3	3:J:357:VAL:HG11	1.91	0.52
3:D:1279:GLN:HB2	3:D:1282:TYR:HB2	1.92	0.52
3:J:1156:LEU:HD13	3:J:1223:LEU:HD12	1.91	0.52
3:J:799:ARG:HB3	3:J:1309:ILE:HG21	1.91	0.52
2:C:400:VAL:HG11	2:C:452:ARG:HD2	1.92	0.52
3:J:528:THR:HG22	3:J:532:GLU:HB2	1.92	0.52
3:J:814:CYS:SG	3:J:895:CYS:CB	2.97	0.52
5:F:548:LEU:HD13	5:F:560:ARG:HE	1.75	0.52
2:C:1086:PRO:HB2	2:C:1212:LEU:HD23	1.92	0.51
3:D:263:SER:HA	5:F:507:MET:HB2	1.91	0.51
2:C:802:VAL:HG21	2:C:1230:MET:HB3	1.92	0.51
2:I:1060:ILE:HG23	2:I:1076:ILE:HD13	1.92	0.51
2:C:148:GLN:HB3	2:C:454:ARG:HB2	1.92	0.51
3:D:492:SER:HB3	3:D:499:ILE:HB	1.92	0.51
5:L:548:LEU:HD13	5:L:560:ARG:HE	1.76	0.51
2:I:447:HIS:HB3	2:I:450:ASN:HD22	1.75	0.51
5:F:151:VAL:HB	5:F:161:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:854:ALA:O	3:J:855:ASP:HB2	2.09	0.51
3:D:450:HIS:HB3	3:D:453:VAL:HG22	1.93	0.51
1:B:89:ALA:HB1	1:B:210:THR:HG23	1.93	0.51
3:J:491:LEU:HA	3:J:498:PRO:HA	1.92	0.51
2:I:1252:SER:HB3	2:I:1259:LEU:HD22	1.93	0.50
3:J:322:ARG:HH21	5:L:510:PRO:HG2	1.76	0.50
3:D:820:ILE:HA	3:D:1227:HIS:CE1	2.46	0.50
3:J:1138:LEU:N	3:J:1139:PRO:HD2	2.26	0.50
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.92	0.50
2:I:672:GLU:HB3	3:J:767:LEU:H	1.76	0.50
2:C:710:VAL:HG13	2:C:717:VAL:HG11	1.93	0.50
3:D:639:VAL:HG13	3:D:722:ILE:HD11	1.94	0.50
3:J:1145:PHE:HB3	3:J:1309:ILE:HD11	1.93	0.50
5:F:110:LEU:HD11	5:F:385:ARG:HD2	1.94	0.50
1:A:27:THR:HG22	1:A:202:VAL:HG22	1.93	0.50
1:A:228:LEU:HD11	1:B:224:LEU:HD23	1.94	0.50
2:C:926:GLY:H	2:C:1056:VAL:HG22	1.77	0.49
2:I:1223:ARG:HH22	3:J:719:PHE:HB2	1.77	0.49
3:D:919:ALA:HA	3:D:1252:HIS:HD1	1.77	0.49
2:I:142:GLU:HB3	2:I:760:ASN:HD21	1.77	0.49
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.93	0.49
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.94	0.49
3:J:1290:ARG:HA	3:J:1294:ALA:HB3	1.94	0.49
3:J:288:PRO:HG2	3:J:291:ILE:HD12	1.93	0.49
3:J:325:LYS:HG3	5:L:508:GLU:HG3	1.94	0.49
3:D:1301:THR:HG21	3:J:1298:VAL:HG13	1.94	0.49
3:J:1311:LYS:HA	3:J:1314:LEU:HD12	1.95	0.49
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.93	0.49
3:D:452:LEU:HB3	3:D:500:ILE:HG23	1.94	0.49
3:D:720:ASN:HD22	3:D:722:ILE:H	1.61	0.48
3:J:903:LEU:HD12	3:J:1252:HIS:HE2	1.78	0.48
3:J:490:ILE:HA	3:J:500:ILE:HD12	1.95	0.48
5:L:96:ASP:N	5:L:97:PRO:HD2	2.27	0.48
3:J:1176:VAL:HG22	3:J:1187:GLU:HG2	1.95	0.48
2:C:476:LYS:HA	2:C:479:LEU:HD12	1.96	0.48
2:C:521:LEU:HD11	2:C:664:GLY:HA2	1.95	0.48
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.94	0.48
4:E:25:ARG:HD2	4:E:64:LEU:HD13	1.95	0.48
2:C:520:PRO:HD2	2:C:788:SER:HB2	1.94	0.48
2:C:660:VAL:HG23	2:C:661:VAL:HG23	1.96	0.48
2:I:681:MET:O	2:I:685:MET:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:844:LYS:HD3	2:I:844:LYS:H	1.79	0.48
5:L:364:ARG:HA	5:L:367:ILE:HD12	1.96	0.48
5:L:397:ARG:HG2	5:L:443:ILE:HD13	1.95	0.48
3:D:490:ILE:HA	3:D:500:ILE:HD12	1.95	0.48
4:K:38:LEU:HD13	4:K:58:LEU:HB3	1.95	0.48
1:B:192:VAL:HG12	1:B:193:GLU:H	1.77	0.48
2:I:808:ASN:HA	3:J:629:PHE:HB3	1.95	0.48
2:C:809:GLY:HA3	3:D:359:PRO:HB3	1.96	0.48
2:I:733:VAL:HG12	2:I:750:ILE:HA	1.96	0.47
3:J:664:ILE:HD12	3:J:685:ILE:HD11	1.96	0.47
3:J:739:GLN:HG2	3:J:744:ARG:HA	1.96	0.47
1:G:27:THR:HG22	1:G:202:VAL:HG22	1.96	0.47
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.94	0.47
3:J:298:MET:SD	5:L:402:LEU:HD22	2.53	0.47
2:C:309:LEU:HD21	2:C:312:ALA:HB2	1.95	0.47
2:C:696:ASP:HB3	2:C:798:GLN:HG3	1.95	0.47
2:C:6:THR:HA	2:C:9:LYS:HE3	1.97	0.47
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.97	0.47
2:C:1292:THR:HG22	2:C:1320:PRO:HG3	1.95	0.47
3:J:1060:VAL:HG22	3:J:1106:ILE:HG12	1.96	0.47
3:D:1375:ALA:HB2	3:J:849:LEU:HB3	1.96	0.47
3:D:294:ASN:HD22	3:D:297:ARG:HH11	1.62	0.47
2:C:804:PHE:HB3	2:C:1100:PRO:HB3	1.97	0.47
2:C:28:LEU:HD22	2:C:527:LYS:HD2	1.96	0.47
5:L:246:GLN:HA	5:L:249:ILE:HD12	1.97	0.47
3:D:450:HIS:HD2	3:D:452:LEU:HB2	1.79	0.47
2:C:1315:MET:HG3	3:D:473:THR:HG21	1.96	0.47
3:D:113:HIS:CD2	3:D:115:TRP:HB2	2.50	0.47
3:D:965:SER:HA	3:D:975:ILE:HA	1.97	0.47
2:I:592:ARG:HB2	2:I:653:MET:HB3	1.97	0.47
3:J:214:ARG:HA	3:J:217:LEU:HD12	1.96	0.47
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.97	0.46
3:D:591:ILE:HG12	3:D:604:MET:HG2	1.97	0.46
2:C:444:ASP:HB3	2:C:447:HIS:HB2	1.97	0.46
3:D:1054:THR:H	3:D:1055:GLY:HA2	1.79	0.46
5:L:407:GLU:HG2	5:L:442:SER:HB2	1.98	0.46
2:C:1287:LEU:HD22	3:D:1357:ILE:HD11	1.96	0.46
3:D:850:LYS:HG3	3:D:877:VAL:HG13	1.98	0.46
1:H:158:ARG:HE	1:H:172:LEU:HD22	1.80	0.46
2:I:1330:ILE:HA	2:I:1333:LEU:HD12	1.96	0.46
2:I:975:ILE:HG12	2:I:1014:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:843:VAL:HG23	3:J:900:GLY:HA2	1.96	0.46
5:L:341:LEU:HA	5:L:344:LEU:HD12	1.96	0.46
2:C:933:VAL:HG13	2:C:1050:VAL:HG22	1.97	0.46
3:D:888:CYS:SG	3:D:898:CYS:SG	3.14	0.46
2:I:1252:SER:HA	5:L:524:GLU:HA	1.98	0.46
3:D:331:ILE:HG23	3:D:338:PHE:HB2	1.96	0.46
3:D:610:ARG:HG2	3:D:866:GLU:HB2	1.98	0.46
3:J:1036:ARG:HB2	3:J:1079:LYS:HB3	1.96	0.46
3:D:450:HIS:CD2	3:D:452:LEU:HB2	2.50	0.46
3:D:814:CYS:CB	3:D:895:CYS:SG	3.01	0.46
1:H:57:THR:HG21	1:H:147:GLN:HE21	1.80	0.46
2:I:151:ARG:HH22	2:I:175:ARG:HH11	1.64	0.46
5:F:582:VAL:HG12	5:F:583:THR:H	1.81	0.46
3:J:530:PRO:HG3	3:J:552:ILE:HG22	1.97	0.46
3:D:1296:GLY:O	3:D:1297:LYS:HG2	2.15	0.46
1:G:134:THR:HG23	2:I:773:LEU:HD21	1.98	0.46
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.97	0.46
3:D:1238:GLN:HE21	3:D:1253:ILE:HD11	1.80	0.46
5:F:227:GLN:HA	5:F:230:VAL:HG12	1.97	0.46
2:I:883:LEU:HD21	2:I:1054:LEU:HD11	1.98	0.46
3:J:925:GLU:HB3	3:J:926:PRO:HD3	1.98	0.46
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.88	0.45
5:F:290:LEU:HD22	5:F:333:VAL:HG21	1.98	0.45
3:J:561:GLY:HA2	3:J:562:GLU:HA	1.65	0.45
2:I:1280:ALA:HB1	3:J:918:ILE:HG12	1.98	0.45
3:D:1069:ALA:HA	3:D:1072:LYS:HE2	1.97	0.45
3:D:152:THR:HG21	3:D:176:PHE:HB2	1.99	0.45
3:D:799:ARG:HG2	3:D:1309:ILE:HG21	1.99	0.45
2:I:1296:ASP:HB3	2:I:1321:GLU:H	1.82	0.45
2:I:74:ARG:HH21	2:I:97:ARG:HD2	1.80	0.45
5:L:348:GLU:HG2	5:L:354:THR:HA	1.98	0.45
2:C:533:LEU:HD21	2:C:571:LEU:HD13	1.98	0.45
3:D:1221:LEU:HD22	3:D:1306:LEU:HB2	1.97	0.45
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.99	0.45
3:J:749:LYS:HE3	3:J:755:ILE:HA	1.97	0.45
3:J:93:THR:HG22	3:J:94:GLN:H	1.80	0.45
1:G:231:PHE:HB3	1:H:218:ARG:HA	1.98	0.45
3:J:450:HIS:HB3	3:J:453:VAL:HG22	1.98	0.45
3:D:1220:ILE:HG23	3:D:1224:ARG:HD2	1.98	0.45
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.98	0.45
2:I:789:THR:HG22	2:I:794:LEU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:268:LEU:HG	3:J:324:LEU:HD22	1.98	0.45
2:C:406:ASN:HB3	2:C:411:ARG:HB2	1.97	0.45
3:D:1046:ILE:HD12	3:D:1059:LEU:HD22	1.99	0.45
3:D:298:MET:HG3	5:F:402:LEU:HD22	1.99	0.45
5:F:120:ALA:HA	5:F:123:ILE:HD12	1.98	0.45
2:I:397:LEU:HB3	2:I:401:GLY:HA3	1.98	0.45
3:J:1158:GLU:HA	3:J:1223:LEU:HD21	1.98	0.45
3:J:423:LEU:HD21	3:J:447:ILE:HD13	1.99	0.45
5:L:120:ALA:HA	5:L:123:ILE:HD12	1.99	0.45
2:C:101:ARG:HB3	2:C:118:LYS:HG3	1.99	0.45
3:D:886:VAL:HG11	3:D:1230:THR:HG21	1.99	0.45
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.83	0.45
2:C:802:VAL:HG22	2:C:1096:ILE:HD11	1.99	0.45
3:D:114:ILE:HD11	3:D:311:ARG:HB2	1.98	0.45
3:D:417:ARG:HG2	3:D:418:GLU:HG2	1.99	0.45
3:D:561:GLY:HA2	3:D:562:GLU:HA	1.68	0.45
1:A:192:VAL:HG12	1:A:194:GLN:H	1.81	0.44
1:A:82:LEU:HD11	1:A:171:LEU:HD13	1.99	0.44
2:C:447:HIS:CD2	2:C:449:GLY:H	2.32	0.44
3:D:930:LEU:HD23	3:D:1244:GLN:HG3	1.97	0.44
2:I:560:PRO:HB2	3:J:776:THR:HG21	1.98	0.44
3:D:123:ARG:HD2	3:D:1337:VAL:HG21	1.99	0.44
2:I:101:ARG:HB3	2:I:118:LYS:HG3	2.00	0.44
3:D:1276:GLU:HB3	3:D:1277:GLY:H	1.63	0.44
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.99	0.44
2:I:462:ASN:OD1	2:I:463:GLN:N	2.50	0.44
3:J:558:ASP:HB2	3:J:563:LEU:H	1.81	0.44
3:J:910:ASN:ND2	4:K:16:ARG:H	2.16	0.44
2:C:1061:GLN:HB2	2:C:1062:PRO:HD2	1.98	0.44
5:F:341:LEU:HD23	5:F:345:GLN:HB2	1.99	0.44
2:I:26:TYR:HB3	2:I:29:SER:HB3	2.00	0.44
3:J:1046:ILE:HD12	3:J:1059:LEU:HD22	1.99	0.44
3:J:492:SER:HB3	3:J:499:ILE:HB	2.00	0.44
2:C:858:GLY:HA2	2:C:859:GLU:HA	1.64	0.44
1:G:159:ILE:HA	1:G:166:ARG:HH12	1.83	0.44
2:I:1074:GLY:HA2	3:J:462:ASP:HA	1.99	0.44
5:L:426:LYS:HG3	5:L:428:SER:H	1.82	0.44
1:B:25:LYS:HG2	1:B:204:GLU:HG2	1.99	0.44
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	2.00	0.44
3:D:1036:ARG:HB2	3:D:1079:LYS:HB3	1.99	0.44
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.89	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:804:PHE:HB3	2:I:1100:PRO:HB3	1.98	0.44
2:I:870:ILE:HD11	2:I:944:ARG:HG2	1.99	0.44
1:A:29:GLU:HB2	1:A:30:PRO:HA	2.00	0.44
2:C:559:CYS:HB2	2:C:662:SER:HB2	1.99	0.44
3:D:1348:LYS:HA	3:D:1348:LYS:HE3	2.00	0.44
5:F:551:LEU:HB3	5:F:555:GLU:HB2	1.99	0.44
3:J:1212:ASP:HA	3:J:1213:GLY:HA3	1.71	0.44
3:J:1178:THR:HA	3:J:1179:PRO:HD3	1.87	0.44
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.88	0.44
3:J:1284:ARG:HA	3:J:1287:ILE:HG22	2.00	0.43
2:C:1065:LYS:HD3	2:C:1235:LEU:HD11	2.00	0.43
3:J:452:LEU:HB3	3:J:500:ILE:HG23	2.01	0.43
2:C:1124:ILE:HG12	2:C:1201:LEU:HD23	2.00	0.43
3:D:1262:ARG:O	3:D:1263:LYS:HB2	2.19	0.43
1:G:45:ARG:HH12	2:I:1084:ASP:HB3	1.83	0.43
2:C:385:PHE:HA	2:C:388:LEU:HD12	2.00	0.43
3:D:325:LYS:HD3	3:D:329:ASP:HB3	2.00	0.43
5:F:460:ILE:HA	5:F:463:LEU:HD12	2.00	0.43
3:D:863:LEU:HD11	3:D:908:ILE:HB	2.00	0.43
1:B:46:ILE:HD11	1:B:224:LEU:HD13	1.99	0.43
3:J:118:LYS:HE3	3:J:312:ARG:HG2	1.99	0.43
2:I:813:GLU:HG3	3:J:504:GLN:HE22	1.83	0.43
1:B:47:LEU:HD22	1:B:180:VAL:HG21	2.01	0.43
3:D:358:GLY:HA3	3:D:361:LEU:HD12	2.00	0.43
3:D:428:THR:HG22	3:D:433:GLY:HA3	2.01	0.43
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.99	0.43
2:I:174:ALA:HB2	2:I:432:LEU:HD13	2.01	0.43
3:D:490:ILE:HD12	3:D:491:LEU:HG	2.01	0.43
2:I:1058:ARG:HD2	2:I:1238:LEU:HD13	2.00	0.43
2:I:189:ASP:HB2	2:I:190:PRO:HD2	2.01	0.43
2:I:594:VAL:HG22	2:I:599:VAL:HG13	2.01	0.43
2:I:813:GLU:HB3	3:J:461:PHE:HD2	1.84	0.43
2:C:883:LEU:HD21	2:C:1054:LEU:HD11	2.00	0.43
3:J:1165:PHE:HD2	3:J:1200:GLU:HB3	1.83	0.43
5:L:126:GLY:HA3	5:L:372:ALA:HB2	2.01	0.43
2:C:100:LEU:HD13	2:C:493:ILE:HD12	2.01	0.43
2:C:59:ILE:HD12	2:C:472:GLU:HB2	2.01	0.43
2:C:75:LEU:HB3	2:C:76:GLY:H	1.71	0.43
3:D:646:ILE:HD11	3:D:764:ARG:HG2	2.01	0.43
2:I:1109:ILE:HD11	3:J:740:LEU:HD22	2.01	0.43
2:I:636:CYS:HB2	2:I:645:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1348:LYS:HE3	3:J:1348:LYS:HA	2.01	0.43
3:J:647:PRO:HG2	3:J:650:LYS:HB2	2.01	0.43
2:C:524:ILE:HD12	2:C:708:VAL:HG13	2.01	0.42
5:F:444:ALA:HB1	5:F:457:ILE:HG13	2.00	0.42
1:G:51:MET:HA	1:G:52:PRO:HD3	1.89	0.42
3:J:121:PRO:HG2	3:J:126:LEU:HD11	1.99	0.42
3:J:506:VAL:HG13	3:J:628:GLY:HA3	2.00	0.42
3:D:890:THR:OG1	3:D:895:CYS:SG	2.59	0.42
2:I:817:LEU:HB2	2:I:1097:VAL:HB	2.00	0.42
3:J:532:GLU:HA	3:J:535:ARG:HD3	2.00	0.42
1:B:193:GLU:HG2	3:D:406:ALA:HB1	2.00	0.42
3:J:334:LYS:HA	3:J:339:ARG:HD3	2.02	0.42
1:B:27:THR:HG22	1:B:202:VAL:HG22	2.02	0.42
2:C:1151:LEU:HD21	2:C:1201:LEU:HD13	2.01	0.42
2:C:1142:ARG:HD3	2:C:1162:SER:HB3	2.01	0.42
2:C:838:CYS:HB2	2:C:918:LEU:HD22	2.01	0.42
3:D:974:VAL:HG22	3:D:1002:VAL:HG22	2.01	0.42
3:J:1000:GLY:HA2	3:J:1028:ILE:HD11	2.00	0.42
2:C:1330:ILE:HA	2:C:1333:LEU:HD12	2.02	0.42
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.34	0.42
1:G:167:PRO:HD2	1:G:170:ARG:HG3	2.00	0.42
1:B:190:ALA:HB2	1:B:200:LYS:HB3	2.01	0.42
3:D:424:ASN:HB3	3:D:467:ALA:HB3	2.01	0.42
3:D:749:LYS:HE2	3:D:755:ILE:HG12	2.01	0.42
2:I:148:GLN:HB3	2:I:454:ARG:HB2	2.01	0.42
2:I:811:ASN:HA	2:I:815:SER:HB2	2.01	0.42
3:J:1054:THR:N	3:J:1055:GLY:HA2	2.35	0.42
2:C:836:LEU:HD12	2:C:1054:LEU:HD13	2.00	0.42
2:C:135:THR:HG22	2:C:144:VAL:HG22	2.01	0.42
2:C:232:ILE:HD11	2:C:333:ILE:HD11	2.00	0.42
2:I:10:ARG:HH12	2:I:790:ASP:HB3	1.84	0.42
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	2.02	0.42
3:J:114:ILE:HD12	3:J:304:ASP:HB3	2.02	0.42
2:C:1196:LYS:HA	2:C:1199:LEU:HD12	2.02	0.42
3:D:964:LYS:HB2	3:D:977:SER:HB3	2.02	0.42
1:H:44:ARG:NH1	3:J:538:ARG:HB3	2.35	0.42
2:I:1315:MET:HG3	3:J:473:THR:HG21	2.01	0.42
2:I:858:GLY:HA2	2:I:859:GLU:HA	1.63	0.42
3:J:426:ALA:HA	3:J:427:PRO:HA	1.85	0.42
2:I:1313:HIS:HB2	3:J:474:LEU:HD13	2.01	0.42
5:L:324:LYS:H	5:L:327:SER:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:268:LEU:HG	3:D:324:LEU:HD22	2.02	0.41
2:I:1319:MET:HA	2:I:1320:PRO:HD3	1.93	0.41
2:I:972:PHE:HA	2:I:975:ILE:HD12	2.01	0.41
3:J:358:GLY:HA3	3:J:361:LEU:HD12	2.02	0.41
5:L:399:LEU:HG	5:L:447:ALA:HB2	2.02	0.41
3:D:1054:THR:CG2	3:D:1055:GLY:HA2	2.50	0.41
3:D:1307:LEU:HB3	3:D:1311:LYS:HB3	2.03	0.41
5:F:364:ARG:HA	5:F:367:ILE:HD12	2.01	0.41
5:F:509:THR:HA	5:F:510:PRO:HD3	1.91	0.41
2:I:691:PRO:HB3	2:I:788:SER:HB3	2.02	0.41
3:J:242:LEU:HA	3:J:243:PRO:HD2	1.96	0.41
2:C:67:GLU:HG2	2:C:105:TYR:HE1	1.84	0.41
3:D:826:ILE:HG12	3:D:831:VAL:HG22	2.01	0.41
1:G:86:LYS:HE2	1:G:174:ASP:H	1.85	0.41
3:J:1357:ILE:C	3:J:1359:ALA:H	2.23	0.41
2:C:689:ALA:HA	2:C:1235:LEU:HA	2.03	0.41
3:D:523:GLU:HA	3:D:548:VAL:HG22	2.02	0.41
3:J:46:TYR:HB2	5:L:500:ILE:HG21	2.01	0.41
2:C:1339:LEU:HD23	3:D:20:ILE:HG12	2.01	0.41
2:C:242:VAL:HA	2:C:243:PRO:HD3	1.93	0.41
3:J:975:ILE:HD12	3:J:1001:ALA:HB3	2.03	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.90	0.41
1:A:227:GLN:HB3	1:B:39:LEU:HD11	2.02	0.41
2:C:22:LEU:HD13	2:C:603:ILE:HD13	2.02	0.41
2:C:811:ASN:HA	2:C:815:SER:HB2	2.03	0.41
3:D:1054:THR:N	3:D:1055:GLY:HA2	2.34	0.41
1:G:46:ILE:HD11	1:G:224:LEU:HD13	2.02	0.41
2:I:22:LEU:HD13	2:I:603:ILE:HD13	2.02	0.41
2:C:1064:ASP:HB2	2:C:1076:ILE:HD12	2.03	0.41
2:C:122:VAL:HG13	2:C:490:GLN:HG3	2.02	0.41
2:C:612:GLY:HA2	2:C:639:LYS:HA	2.02	0.41
2:I:138:ILE:HB	2:I:143:ARG:HD3	2.03	0.41
1:B:51:MET:HA	1:B:52:PRO:HD3	1.82	0.41
4:E:38:LEU:HD13	4:E:58:LEU:HB3	2.03	0.41
5:F:407:GLU:HA	5:F:410:ILE:HD12	2.03	0.41
1:H:46:ILE:HD11	1:H:224:LEU:HD13	2.03	0.41
2:I:24:VAL:HA	2:I:25:PRO:HD3	1.94	0.41
3:J:808:VAL:HG21	3:J:1347:LEU:HD21	2.03	0.41
5:L:344:LEU:HA	5:L:347:ILE:HD12	2.02	0.41
2:C:592:ARG:HB2	2:C:653:MET:HB3	2.03	0.41
2:I:836:LEU:HD12	2:I:1054:LEU:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.95	0.41
2:I:127:ILE:HA	2:I:128:PRO:HD3	1.95	0.41
1:B:11:PRO:HG3	1:B:31:LEU:HG	2.03	0.40
2:C:1117:LEU:HD13	2:C:1195:ILE:HG12	2.03	0.40
2:C:744:GLY:HA2	2:C:1013:GLN:HB3	2.03	0.40
5:F:520:GLY:HA2	5:F:523:ILE:HD12	2.03	0.40
5:F:548:LEU:HA	5:F:551:LEU:HD12	2.02	0.40
1:A:78:ILE:HA	1:A:81:ILE:HD12	2.03	0.40
3:D:242:LEU:HA	3:D:243:PRO:HD2	1.99	0.40
3:D:85:CYS:HB3	3:D:89:GLY:H	1.86	0.40
1:G:134:THR:HA	2:I:773:LEU:HD11	2.04	0.40
5:L:491:GLU:HA	5:L:494:ILE:HD12	2.03	0.40
3:D:275:ARG:HH12	3:D:298:MET:HE3	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	225/329 (68%)	216 (96%)	6 (3%)	3 (1%)	12	48
1	B	225/329 (68%)	213 (95%)	12 (5%)	0	100	100
1	G	225/329 (68%)	214 (95%)	10 (4%)	1 (0%)	34	72
1	H	225/329 (68%)	217 (96%)	7 (3%)	1 (0%)	34	72
2	C	1338/1342 (100%)	1208 (90%)	107 (8%)	23 (2%)	9	44
2	I	1338/1342 (100%)	1186 (89%)	131 (10%)	21 (2%)	9	45
3	D	1336/1416 (94%)	1206 (90%)	110 (8%)	20 (2%)	10	46
3	J	1332/1416 (94%)	1207 (91%)	111 (8%)	14 (1%)	14	52
4	E	88/90 (98%)	82 (93%)	5 (6%)	1 (1%)	14	52
4	K	88/90 (98%)	83 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	477/628 (76%)	432 (91%)	36 (8%)	9 (2%)	8	41
5	L	477/628 (76%)	442 (93%)	27 (6%)	8 (2%)	9	44
All	All	7374/8268 (89%)	6706 (91%)	567 (8%)	101 (1%)	11	47

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	488	MET
2	C	489	PRO
2	C	555	TYR
2	C	569	ILE
5	F	243	ALA
5	F	553	ALA
2	I	65	ASN
2	I	555	TYR
3	J	316	ILE
2	C	373	GLY
2	C	730	SER
2	C	791	LEU
3	D	527	LEU
3	D	891	ASP
3	D	896	ALA
3	D	1309	ILE
2	I	120	GLN
2	I	399	ALA
3	J	53	ARG
3	J	178	ALA
3	J	286	ALA
3	J	1309	ILE
5	L	243	ALA
2	C	43	PRO
2	C	625	GLU
2	C	868	SER
2	C	892	GLU
2	C	1004	ASP
2	C	1153	ALA
2	C	1263	ALA
3	D	53	ARG
3	D	174	ASP
3	D	286	ALA
3	D	463	GLY

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Mol	Chain	Res	Type
3	D	1167	LYS
3	D	1179	PRO
3	D	1297	LYS
4	E	35	LYS
5	F	166	VAL
5	F	514	ASP
2	I	165	HIS
2	I	626	GLU
2	I	730	SER
2	I	938	GLY
3	J	463	GLY
3	J	527	LEU
5	L	166	VAL
5	L	476	ARG
1	A	51	MET
2	C	134	GLY
2	C	455	SER
2	C	669	PRO
2	C	1103	VAL
2	C	1155	VAL
2	C	1261	GLY
3	D	122	SER
3	D	233	LYS
3	D	546	ALA
5	F	160	ASP
5	F	398	GLY
1	G	165	GLU
1	H	181	GLU
2	I	20	GLN
2	I	244	GLU
2	I	488	MET
2	I	922	ASN
2	I	1103	VAL
2	I	1236	ASN
3	J	122	SER
3	J	233	LYS
3	J	1183	SER
5	L	160	ASP
1	A	50	SER
1	A	165	GLU
2	C	165	HIS
3	D	852	GLY

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Mol	Chain	Res	Type
3	D	857	LEU
3	D	1296	GLY
5	F	516	ASP
2	I	489	PRO
2	I	1135	GLN
3	J	546	ALA
3	J	564	VAL
5	L	113	ARG
5	L	155	GLU
2	C	879	GLY
5	F	263	PRO
5	F	447	ALA
2	I	545	PHE
2	I	596	ASP
2	I	879	GLY
3	D	1185	PRO
2	I	134	GLY
3	J	852	GLY
2	I	373	GLY
5	L	263	PRO
2	C	939	VAL
3	D	150	GLY
3	D	522	GLY
5	L	398	GLY
3	J	1270	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	195/286 (68%)	192 (98%)	3 (2%)	65	80
1	B	195/286 (68%)	195 (100%)	0	100	100
1	G	195/286 (68%)	191 (98%)	4 (2%)	53	71
1	H	195/286 (68%)	193 (99%)	2 (1%)	76	86
2	C	1155/1157 (100%)	1133 (98%)	22 (2%)	57	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1155/1157 (100%)	1122 (97%)	33 (3%)	42	64
3	D	1123/1177 (95%)	1098 (98%)	25 (2%)	52	70
3	J	1120/1177 (95%)	1090 (97%)	30 (3%)	44	66
4	E	74/74 (100%)	72 (97%)	2 (3%)	44	66
4	K	74/74 (100%)	73 (99%)	1 (1%)	67	80
5	F	427/554 (77%)	419 (98%)	8 (2%)	57	74
5	L	427/554 (77%)	415 (97%)	12 (3%)	43	65
All	All	6335/7068 (90%)	6193 (98%)	142 (2%)	52	70

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ASP
1	A	79	LEU
1	A	197	ASP
2	C	23	ASP
2	C	60	GLN
2	C	149	LEU
2	C	161	LYS
2	C	300	ASP
2	C	403	MET
2	C	476	LYS
2	C	483	ASP
2	C	575	LEU
2	C	596	ASP
2	C	632	ASP
2	C	737	ASN
2	C	794	LEU
2	C	799	ASN
2	C	844	LYS
2	C	890	LYS
2	C	912	ASP
2	C	1029	LEU
2	C	1037	THR
2	C	1042	LEU
2	C	1082	ILE
2	C	1171	ARG
3	D	28	ASP
3	D	93	THR
3	D	223	LEU

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Mol	Chain	Res	Type
3	D	229	GLN
3	D	267	ASP
3	D	275	ARG
3	D	289	ASP
3	D	300	GLN
3	D	460	ASP
3	D	515	ARG
3	D	562	GLU
3	D	571	ASP
3	D	649	LYS
3	D	699	ASP
3	D	895	CYS
3	D	898	CYS
3	D	975	ILE
3	D	1054	THR
3	D	1073	ASP
3	D	1192	LYS
3	D	1193	TRP
3	D	1262	ARG
3	D	1266	ILE
3	D	1305	ASP
3	D	1348	LYS
4	E	18	ASP
4	E	46	THR
5	F	105	MET
5	F	313	ASP
5	F	330	LEU
5	F	341	LEU
5	F	402	LEU
5	F	403	ASP
5	F	507	MET
5	F	582	VAL
1	G	77	ASP
1	G	96	ASP
1	G	120	ASP
1	G	165	GLU
1	H	96	ASP
1	H	174	ASP
2	I	13	LYS
2	I	132	ASP
2	I	142	GLU
2	I	161	LYS

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Mol	Chain	Res	Type
2	I	185	ASP
2	I	275	ARG
2	I	331	LYS
2	I	439	LYS
2	I	473	ARG
2	I	479	LEU
2	I	568	ASN
2	I	575	LEU
2	I	596	ASP
2	I	632	ASP
2	I	648	ASP
2	I	711	ASP
2	I	749	ASP
2	I	844	LYS
2	I	866	ASP
2	I	873	ILE
2	I	886	LYS
2	I	890	LYS
2	I	912	ASP
2	I	940	GLU
2	I	950	GLU
2	I	990	ASP
2	I	1042	LEU
2	I	1082	ILE
2	I	1160	ASP
2	I	1203	ASP
2	I	1219	GLU
2	I	1288	GLN
2	I	1304	MET
3	J	22	ILE
3	J	93	THR
3	J	127	LEU
3	J	132	LEU
3	J	134	ASP
3	J	156	ARG
3	J	223	LEU
3	J	227	PHE
3	J	229	GLN
3	J	252	LEU
3	J	264	ASP
3	J	267	ASP
3	J	300	GLN

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Mol	Chain	Res	Type
3	J	317	THR
3	J	460	ASP
3	J	515	ARG
3	J	551	ARG
3	J	579	LEU
3	J	649	LYS
3	J	837	ASP
3	J	881	LYS
3	J	898	CYS
3	J	954	ASN
3	J	1054	THR
3	J	1087	ASP
3	J	1156	LEU
3	J	1268	ASN
3	J	1273	ASP
3	J	1305	ASP
3	J	1348	LYS
4	K	46	THR
5	L	96	ASP
5	L	105	MET
5	L	161	LEU
5	L	330	LEU
5	L	341	LEU
5	L	402	LEU
5	L	451	ARG
5	L	473	GLU
5	L	492	ASP
5	L	493	LYS
5	L	587	ILE
5	L	603	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	41	ASN
2	C	447	HIS
2	C	490	GLN
2	C	618	GLN
2	C	658	GLN
2	C	766	ASN
2	C	824	GLN
2	C	856	ASN

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Mol	Chain	Res	Type
2	C	1209	GLN
3	D	113	HIS
3	D	294	ASN
3	D	300	GLN
3	D	720	ASN
3	D	1227	HIS
3	D	1238	GLN
3	D	1249	ASN
3	D	1289	ASN
4	E	70	GLN
5	F	406	GLN
1	G	75	GLN
1	H	41	ASN
1	H	147	GLN
2	I	46	GLN
2	I	447	HIS
2	I	450	ASN
2	I	517	GLN
2	I	658	GLN
2	I	760	ASN
2	I	799	ASN
2	I	1312	ASN
3	J	113	HIS
3	J	294	ASN
3	J	488	ASN
3	J	702	GLN
3	J	1023	HIS
3	J	1227	HIS
3	J	1279	GLN
5	L	129	GLN
5	L	210	ASN
5	L	406	GLN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 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	$\# Z > 2$
7	G4P	K	101	-	30,38,38	1.30	3 (10%)	43,61,61	1.84	8 (18%)
7	G4P	D	2001	-	30,38,38	1.40	4 (13%)	43,61,61	1.92	8 (18%)

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
7	G4P	K	101	-	-	1/23/43/43	0/3/3/3
7	G4P	D	2001	-	-	1/23/43/43	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	101	G4P	C6-C5	4.46	1.49	1.41
7	D	2001	G4P	C6-C5	3.82	1.47	1.41
7	K	101	G4P	O4'-C1'	3.17	1.45	1.41
7	D	2001	G4P	O4'-C1'	3.04	1.45	1.41
7	D	2001	G4P	C5-C4	2.64	1.47	1.40
7	K	101	G4P	C5-C4	2.38	1.47	1.40
7	D	2001	G4P	PB-O2B	-2.13	1.46	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	101	G4P	C2-N3-C4	5.10	121.18	115.36
7	D	2001	G4P	C2-N3-C4	4.90	120.96	115.36
7	D	2001	G4P	PA-O3A-PB	-4.53	117.28	132.83
7	K	101	G4P	C6-N1-C2	3.89	122.11	115.93
7	D	2001	G4P	C6-N1-C2	3.78	121.94	115.93
7	K	101	G4P	PC-O3C-PD	-3.76	119.91	132.83
7	K	101	G4P	C6-C5-C4	-3.71	117.26	120.80
7	D	2001	G4P	N3-C2-N1	-3.69	122.30	127.22
7	D	2001	G4P	PC-O3C-PD	-3.68	120.21	132.83
7	K	101	G4P	PA-O3A-PB	-3.65	120.30	132.83
7	K	101	G4P	C5-C6-N1	-3.65	118.44	123.43
7	D	2001	G4P	C6-C5-C4	-3.61	117.36	120.80
7	D	2001	G4P	C4-C5-N7	-3.55	105.70	109.40
7	K	101	G4P	N3-C2-N1	-3.51	122.55	127.22
7	D	2001	G4P	C5-C6-N1	-3.22	119.03	123.43
7	K	101	G4P	C4-C5-N7	-2.81	106.47	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	101	G4P	PB-O3A-PA-O1A
7	D	2001	G4P	PB-O3A-PA-O1A

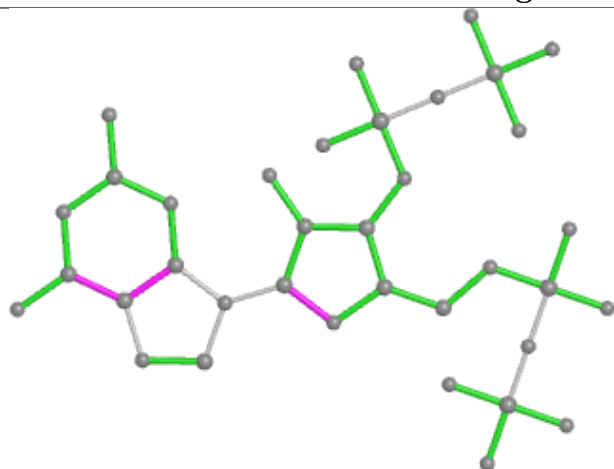
There are no ring outliers.

1 monomer is involved in 1 short contact:

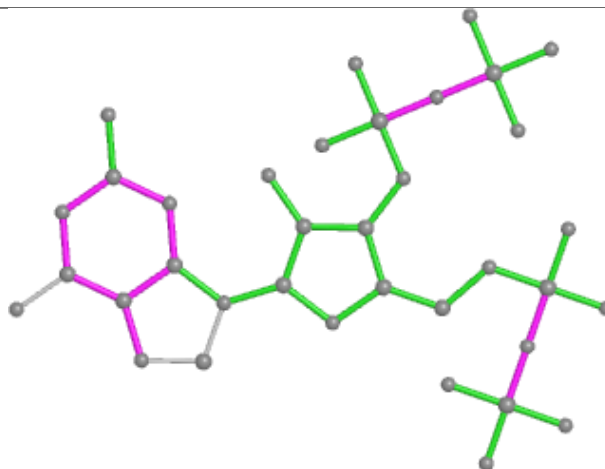
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	2001	G4P	1	0

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.

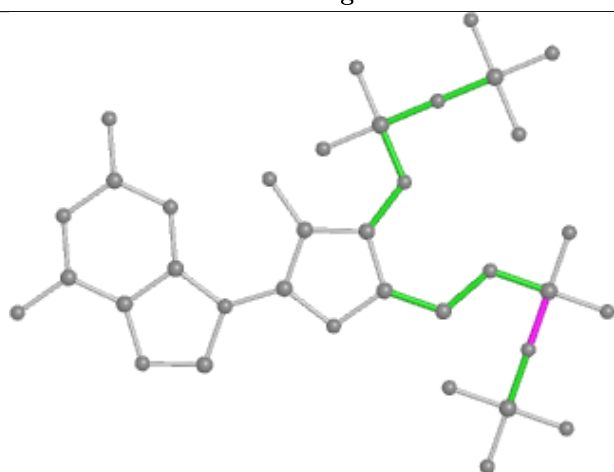
Ligand G4P K 101



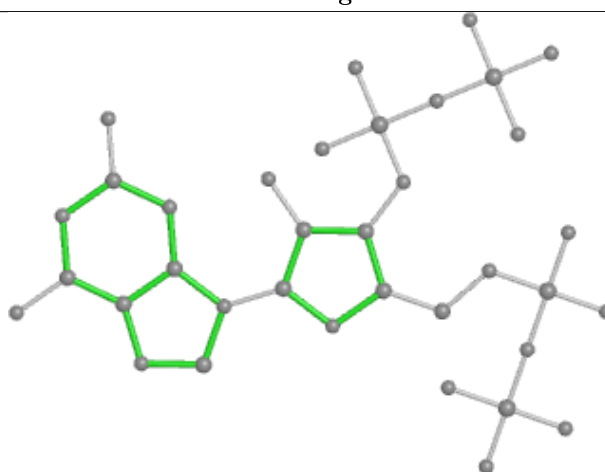
Bond lengths



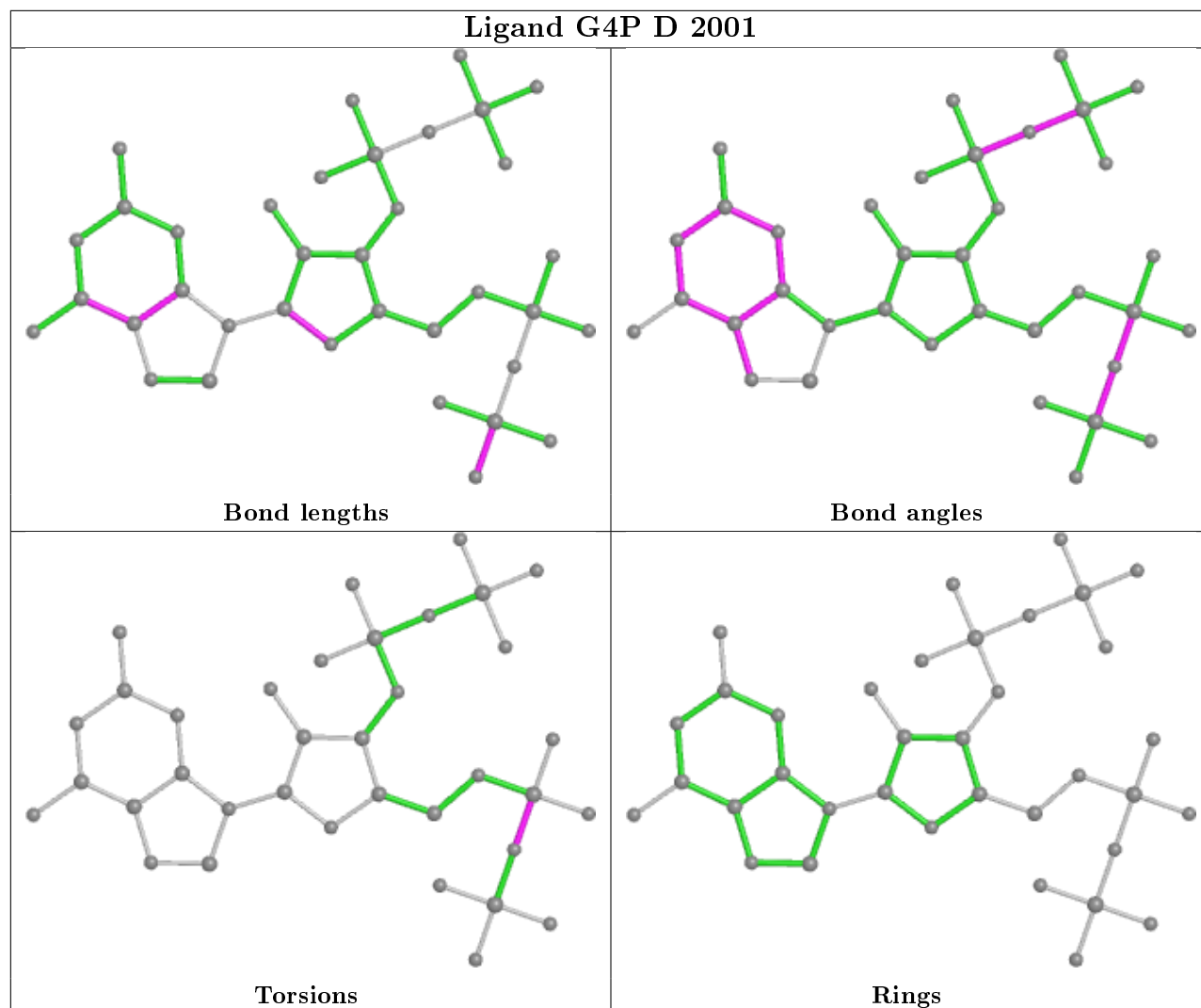
Bond angles



Torsions



Rings



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, 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	227/329 (68%)	-0.14	1 (0%) 92 87	148, 217, 322, 411	0
1	B	227/329 (68%)	-0.00	5 (2%) 62 52	155, 276, 386, 464	0
1	G	227/329 (68%)	-0.09	4 (1%) 68 59	195, 272, 381, 487	0
1	H	227/329 (68%)	0.30	16 (7%) 16 13	209, 313, 434, 551	0
2	C	1340/1342 (99%)	-0.13	31 (2%) 60 51	116, 219, 400, 608	0
2	I	1340/1342 (99%)	-0.03	43 (3%) 47 37	158, 257, 405, 600	0
3	D	1342/1416 (94%)	0.29	128 (9%) 8 8	114, 234, 543, 696	0
3	J	1338/1416 (94%)	0.38	127 (9%) 8 8	158, 266, 556, 725	0
4	E	90/90 (100%)	-0.12	0 100 100	147, 230, 311, 405	0
4	K	90/90 (100%)	0.73	14 (15%) 2 2	217, 322, 517, 666	0
5	F	481/628 (76%)	0.03	25 (5%) 27 23	153, 297, 481, 614	0
5	L	481/628 (76%)	0.12	27 (5%) 24 21	182, 318, 469, 601	0
All	All	7410/8268 (89%)	0.11	421 (5%) 23 20	114, 258, 482, 725	0

All (421) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	1073	ASP	22.8
3	J	1118	GLY	18.5
3	J	1125	PRO	17.7
3	D	983	LYS	16.8
3	J	1057	SER	12.1
3	D	1122	ALA	11.0
5	L	158	LEU	10.8
3	D	1121	LEU	10.5
3	J	1119	ASP	10.1
3	D	1112	GLY	9.7
3	D	854	ALA	9.2

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Mol	Chain	Res	Type	RSRZ
3	J	983	LYS	9.2
3	J	1126	GLN	8.8
3	J	854	ALA	8.8
3	J	1005	LYS	8.8
3	D	1072	LYS	8.7
2	I	265	LYS	8.6
3	J	970	SER	8.6
3	J	855	ASP	8.4
3	D	1120	THR	8.3
3	J	997	VAL	8.2
3	D	1052	GLU	7.8
2	C	254	ASP	7.8
3	J	982	LEU	7.8
3	J	1063	ASP	7.7
3	D	1050	THR	7.6
3	J	991	THR	7.5
3	J	962	ASN	7.4
3	J	1296	GLY	7.3
5	L	156	ALA	7.3
3	D	982	LEU	7.3
3	J	1075	ARG	7.1
3	J	1110	GLU	7.1
1	B	12	ARG	7.0
2	C	250	THR	6.9
3	D	853	THR	6.9
3	D	962	ASN	6.9
3	J	987	GLU	6.8
3	J	1101	LEU	6.8
3	D	1049	GLN	6.7
3	J	756	GLU	6.6
5	L	240	ARG	6.5
3	D	953	LYS	6.5
3	J	1109	LEU	6.5
4	K	89	GLY	6.5
3	D	1115	ILE	6.4
3	J	998	PRO	6.4
2	C	277	LEU	6.3
3	D	855	ASP	6.3
3	D	972	LYS	6.3
3	D	1108	GLN	6.2
2	C	251	ALA	6.2
3	D	963	VAL	6.2

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Mol	Chain	Res	Type	RSRZ
3	D	1089	LEU	6.1
3	J	1117	SER	6.1
3	J	1100	PHE	6.1
3	D	1008	GLY	6.1
3	D	1084	GLN	6.0
3	D	1185	PRO	6.0
3	J	1056	LEU	6.0
3	J	1006	GLY	6.0
3	J	1124	ILE	5.9
3	J	1295	ASN	5.8
4	K	87	ALA	5.8
2	I	987	GLU	5.7
3	J	1001	ALA	5.7
3	D	1004	ALA	5.7
3	D	1126	GLN	5.7
4	K	90	ARG	5.7
3	D	1044	GLN	5.6
3	D	1114	GLN	5.6
3	D	1013	GLY	5.5
3	D	967	VAL	5.5
2	C	230	PHE	5.5
3	D	1109	LEU	5.5
3	J	1042	ASP	5.5
3	D	1086	ASN	5.4
3	D	952	VAL	5.4
3	D	1097	ALA	5.4
3	J	1065	ALA	5.4
3	J	1099	TYR	5.4
3	J	1041	ILE	5.3
3	D	974	VAL	5.3
3	D	1066	GLU	5.3
2	I	264	GLU	5.2
3	D	1048	ARG	5.2
2	I	986	ALA	5.2
3	D	961	SER	5.2
3	J	155	GLU	5.2
5	F	337	VAL	5.1
3	J	969	SER	5.1
3	D	968	ASN	5.1
2	I	720	ARG	5.0
2	C	268	ARG	5.0
2	I	743	PRO	5.0

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Mol	Chain	Res	Type	RSRZ
3	D	1094	ASP	4.9
1	H	161	SER	4.9
2	C	261	VAL	4.9
3	D	1092	GLY	4.9
2	C	252	SER	4.8
3	D	1051	ASP	4.8
3	D	1111	ASP	4.8
3	D	1058	SER	4.8
3	J	1294	ALA	4.8
3	D	1009	GLU	4.8
2	C	1001	GLY	4.8
4	K	88	GLU	4.8
5	L	290	LEU	4.7
5	F	166	VAL	4.7
5	F	168	PRO	4.7
3	D	1006	GLY	4.7
3	J	1062	LEU	4.7
3	D	1029	THR	4.7
2	C	267	ARG	4.7
3	D	1010	GLN	4.7
4	K	86	ILE	4.6
3	D	1295	ASN	4.6
1	H	12	ARG	4.6
3	J	955	LYS	4.6
4	K	84	THR	4.5
3	D	971	GLY	4.5
5	L	159	SER	4.5
3	J	1029	THR	4.5
2	I	981	ALA	4.5
3	J	963	VAL	4.5
5	F	325	PRO	4.4
3	D	852	GLY	4.4
5	F	340	ALA	4.4
3	D	1085	GLY	4.3
2	I	974	ARG	4.3
3	D	966	VAL	4.3
1	H	13	LEU	4.3
3	D	212	THR	4.3
2	I	281	ASP	4.3
3	D	1031	VAL	4.3
3	J	1187	GLU	4.3
3	J	1086	ASN	4.2

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Mol	Chain	Res	Type	RSRZ
3	D	991	THR	4.2
3	D	1045	THR	4.2
3	J	1107	VAL	4.2
2	I	980	VAL	4.2
2	I	970	GLY	4.2
3	D	1087	ASP	4.2
2	I	979	LEU	4.2
3	J	1031	VAL	4.1
3	D	973	LEU	4.1
3	J	1044	GLN	4.1
3	D	1093	THR	4.0
3	D	1065	ALA	4.0
2	I	999	GLU	4.0
3	D	959	LYS	4.0
2	I	120	GLN	4.0
3	J	1104	LYS	4.0
2	C	231	GLU	4.0
5	L	238	LYS	4.0
5	L	239	GLY	4.0
3	D	947	GLU	4.0
2	C	243	PRO	3.9
3	J	849	LEU	3.9
2	C	332	ARG	3.9
3	J	1010	GLN	3.9
5	L	325	PRO	3.9
5	L	157	ARG	3.9
5	F	244	THR	3.9
1	H	164	ASP	3.9
3	J	996	LYS	3.9
3	J	989	GLY	3.9
5	L	155	GLU	3.9
2	C	253	PHE	3.9
3	D	1047	THR	3.8
3	J	990	ARG	3.8
3	D	1063	ASP	3.8
3	J	986	ASP	3.8
3	D	1113	VAL	3.8
3	J	540	GLY	3.8
3	J	1059	LEU	3.8
3	J	1116	SER	3.7
5	F	157	ARG	3.7
3	J	853	THR	3.7

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Mol	Chain	Res	Type	RSRZ
3	J	1105	ALA	3.7
3	D	1090	ILE	3.7
3	D	1110	GLU	3.7
2	I	254	ASP	3.7
3	D	1088	VAL	3.7
3	J	1003	LEU	3.6
3	J	1083	ALA	3.6
4	K	85	ALA	3.6
1	B	170	ARG	3.6
2	C	333	ILE	3.6
3	D	1007	ASP	3.6
2	C	242	VAL	3.6
3	J	1066	GLU	3.6
5	F	167	ASP	3.6
2	C	1000	LEU	3.5
2	I	266	GLY	3.5
3	D	1005	LYS	3.5
3	J	971	GLY	3.5
3	D	1376	GLY	3.4
5	F	238	LYS	3.4
3	D	1375	ALA	3.4
5	F	343	LYS	3.4
2	I	978	VAL	3.4
3	D	1096	PRO	3.4
5	F	260	ARG	3.4
3	D	1057	SER	3.4
3	D	1119	ASP	3.4
3	J	1043	GLY	3.4
2	I	982	GLY	3.3
3	D	1043	GLY	3.3
3	J	1064	SER	3.3
3	J	1203	ARG	3.3
5	F	160	ASP	3.3
3	D	1034	PHE	3.3
3	D	1125	PRO	3.2
3	D	856	ILE	3.2
2	C	540	ARG	3.2
3	J	1061	VAL	3.2
2	C	266	GLY	3.2
3	D	998	PRO	3.2
1	H	162	GLU	3.2
5	F	341	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	193	GLU	3.2
2	C	1002	LEU	3.2
3	D	1064	SER	3.2
3	J	1094	ASP	3.2
3	J	1102	PRO	3.2
3	J	1015	GLU	3.1
2	C	278	GLU	3.1
3	D	984	LEU	3.1
3	J	1152	GLU	3.1
3	D	1082	ASP	3.1
3	J	993	GLU	3.0
3	D	1160	SER	3.0
5	L	317	ASN	3.0
3	J	1045	THR	3.0
2	C	241	LEU	3.0
2	I	190	PRO	3.0
4	K	83	VAL	3.0
3	J	956	GLY	3.0
3	D	975	ILE	3.0
4	K	91	ARG	3.0
5	L	340	ALA	3.0
3	J	1085	GLY	3.0
2	C	276	GLN	3.0
2	I	1178	LYS	3.0
3	D	1169	THR	3.0
3	D	1203	ARG	3.0
3	J	1047	THR	3.0
3	J	586	GLY	2.9
3	J	988	PHE	2.9
2	I	975	ILE	2.9
5	F	242	HIS	2.9
4	K	82	ALA	2.9
3	J	1032	SER	2.9
2	I	1007	LYS	2.9
1	B	13	LEU	2.9
3	D	1273	ASP	2.9
3	J	1084	GLN	2.8
4	K	58	LEU	2.8
2	I	988	LYS	2.8
3	D	1071	GLY	2.8
3	J	1030	GLU	2.8
3	D	1083	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	1123	ARG	2.8
3	J	1202	GLU	2.8
5	F	301	ASN	2.8
3	J	1168	GLU	2.8
5	L	166	VAL	2.8
1	G	194	GLN	2.8
5	L	613	ASP	2.8
2	I	742	TYR	2.8
5	F	163	THR	2.8
3	D	1173	ARG	2.8
2	I	998	LEU	2.8
3	D	1054	THR	2.7
3	J	968	ASN	2.7
5	L	337	VAL	2.7
3	D	1053	LEU	2.7
3	J	213	LYS	2.7
3	J	69	GLU	2.7
2	I	3	TYR	2.7
1	G	6	THR	2.7
2	I	1008	GLN	2.7
3	D	1171	GLY	2.7
3	D	1055	GLY	2.7
3	D	993	GLU	2.7
3	J	1037	PHE	2.7
3	J	1151	LYS	2.7
3	D	1294	ALA	2.7
5	L	421	TYR	2.7
3	D	1014	GLY	2.7
2	I	1010	GLN	2.7
3	J	985	ILE	2.7
3	J	1185	PRO	2.7
1	H	24	ALA	2.7
3	D	1098	GLN	2.7
3	D	960	LEU	2.6
1	G	196	THR	2.6
2	C	282	VAL	2.6
3	J	974	VAL	2.6
2	I	169	LYS	2.6
3	J	995	TYR	2.6
2	I	1018	TYR	2.6
5	F	156	ALA	2.6
3	D	1170	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
5	F	212	ILE	2.6
5	L	236	LYS	2.6
3	J	966	VAL	2.6
2	C	260	LYS	2.6
3	D	1062	LEU	2.6
3	J	1123	ARG	2.6
5	F	306	PHE	2.6
3	D	970	SER	2.6
3	J	289	ASP	2.5
1	H	168	ILE	2.5
3	D	1000	GLY	2.5
3	D	1091	PRO	2.5
3	D	850	LYS	2.5
2	C	272	ARG	2.5
3	D	1016	THR	2.5
1	H	205	MET	2.5
3	D	849	LEU	2.5
3	J	77	ARG	2.5
2	I	280	ASP	2.5
3	J	1068	THR	2.5
1	B	171	LEU	2.5
3	D	964	LYS	2.4
3	D	1278	GLU	2.4
3	J	233	LYS	2.4
3	J	1052	GLU	2.4
5	F	315	TRP	2.4
5	L	137	TYR	2.4
2	I	165	HIS	2.4
3	J	91	GLU	2.4
2	C	621	SER	2.4
3	J	1034	PHE	2.4
2	C	256	GLU	2.4
3	J	1011	VAL	2.4
5	L	343	LYS	2.4
3	J	713	GLU	2.4
5	L	422	ARG	2.4
3	J	1025	MET	2.4
2	I	258	ASN	2.4
3	J	1160	SER	2.4
3	D	981	GLU	2.4
1	H	120	ASP	2.4
5	F	234	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	J	707	ILE	2.3
3	J	1082	ASP	2.3
3	J	1067	ARG	2.3
2	I	234	ASP	2.3
5	F	171	GLU	2.3
5	L	286	LEU	2.3
4	K	30	MET	2.3
3	J	1161	GLY	2.3
1	G	164	ASP	2.3
3	J	1009	GLU	2.3
2	I	740	GLU	2.3
3	J	1194	ARG	2.3
2	I	1000	LEU	2.3
3	J	965	SER	2.3
3	J	1167	LYS	2.3
5	L	241	SER	2.3
2	I	969	ALA	2.3
5	L	566	ASP	2.3
3	D	1074	LEU	2.3
1	H	6	THR	2.3
5	L	472	GLN	2.3
3	D	992	LYS	2.3
3	D	334	LYS	2.2
2	C	576	SER	2.2
3	J	1023	HIS	2.2
2	I	711	ASP	2.2
3	D	1106	ILE	2.2
3	D	806	ASP	2.2
4	K	80	LEU	2.2
1	H	160	HIS	2.2
5	F	159	SER	2.2
3	J	972	LYS	2.2
5	L	420	GLU	2.2
3	J	852	GLY	2.2
3	J	539	SER	2.2
3	D	1172	LYS	2.2
3	D	1166	GLY	2.2
3	J	1098	GLN	2.2
3	J	1004	ALA	2.2
3	J	1111	ASP	2.2
3	J	682	VAL	2.2
1	H	167	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	1118	GLY	2.2
3	D	1116	SER	2.2
1	H	163	GLU	2.1
3	J	954	ASN	2.1
4	K	79	GLU	2.1
3	J	947	GLU	2.1
5	L	344	LEU	2.1
1	A	117	HIS	2.1
3	D	969	SER	2.1
3	J	518	VAL	2.1
1	H	119	GLY	2.1
3	D	1159	ILE	2.1
3	J	216	LYS	2.1
2	I	779	ARG	2.1
3	D	965	SER	2.1
2	I	915	ASP	2.1
3	J	848	VAL	2.1
2	C	1166	ASP	2.1
2	I	780	GLY	2.1
3	D	1296	GLY	2.1
5	L	313	ASP	2.1
1	H	14	VAL	2.0
3	D	1042	ASP	2.0
2	I	1017	GLN	2.0
3	J	1091	PRO	2.0
3	D	1102	PRO	2.0
5	F	165	PHE	2.0
5	F	283	GLN	2.0
3	J	76	LYS	2.0
1	H	121	VAL	2.0
2	C	259	GLY	2.0
2	I	647	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands

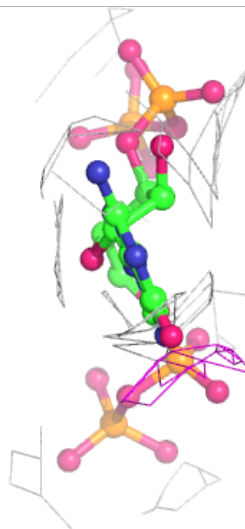
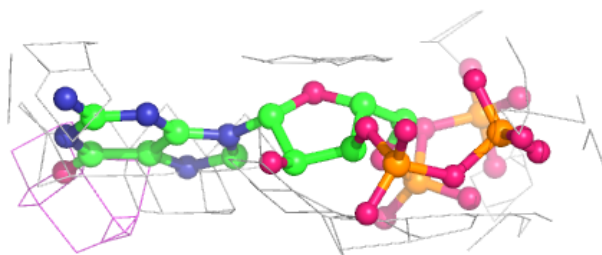
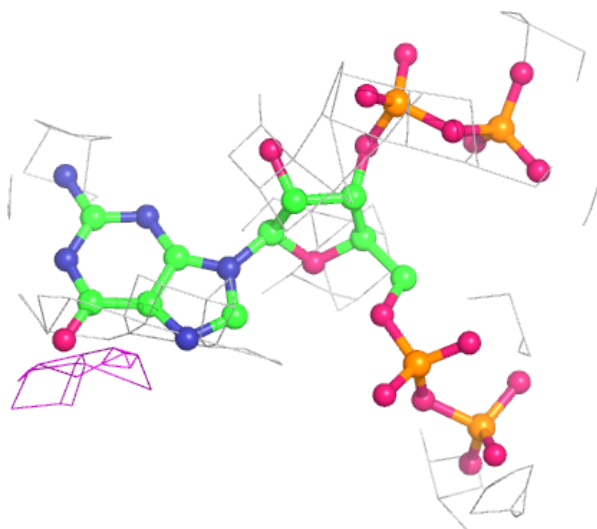
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SR	E	101	1/1	0.69	0.28	328,328,328,328	0
6	SR	I	1401	1/1	0.76	0.39	346,346,346,346	0
7	G4P	K	101	36/36	0.76	0.26	158,256,299,307	0
8	ZN	J	1502	1/1	0.84	0.12	256,256,256,256	0
6	SR	C	1401	1/1	0.85	0.46	303,303,303,303	0
8	ZN	D	2003	1/1	0.88	0.12	245,245,245,245	0
6	SR	A	401	1/1	0.90	0.15	261,261,261,261	0
7	G4P	D	2001	36/36	0.90	0.32	125,188,244,266	0
8	ZN	D	2002	1/1	0.94	0.04	261,261,261,261	0
6	SR	D	2004	1/1	0.94	0.17	288,288,288,288	0
6	SR	F	701	1/1	0.94	0.44	239,239,239,239	0
6	SR	J	1503	1/1	0.95	0.29	322,322,322,322	0
8	ZN	J	1501	1/1	0.96	0.03	249,249,249,249	0
6	SR	C	1402	1/1	0.96	0.62	212,212,212,212	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.

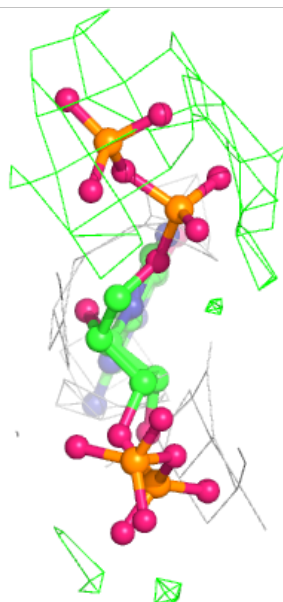
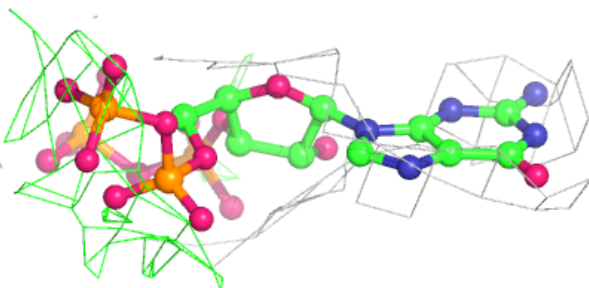
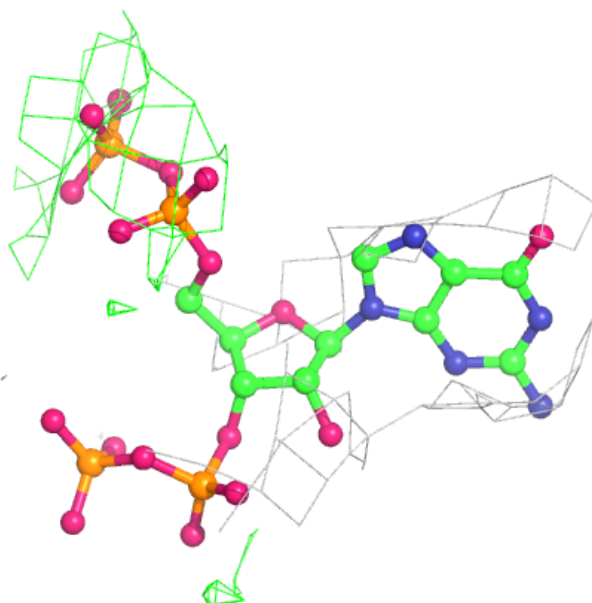
Electron density around G4P K 101:

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



Electron density around G4P D 2001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.