



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:11 PM UTC

PDB ID : 4QWA / pdb_00004qwa
Title : TERNARY CRYSTAL STRUCTURES OF A Y-FAMILY DNA POLYMERASE DPO4 FROM SULFOLOBUS SOLFATARICUS in COMPLEX WITH DNA AND (-)3TC-DP
Authors : Gaur, V.; Suo, Z.
Deposited on : 2014-07-16
Resolution : 2.20 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

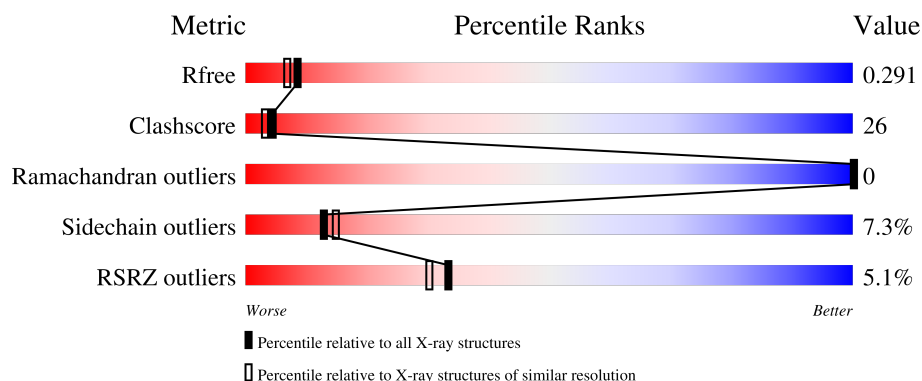
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	349	5% 62% 28% 7% ..
2	C	13	31% 69%
3	D	16	6% 75% 25%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3645 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 polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2743	1760	472	504	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	342	LEU	-	expression tag	UNP Q97W02
A	343	GLU	-	expression tag	UNP Q97W02
A	344	HIS	-	expression tag	UNP Q97W02
A	345	HIS	-	expression tag	UNP Q97W02
A	346	HIS	-	expression tag	UNP Q97W02
A	347	HIS	-	expression tag	UNP Q97W02
A	348	HIS	-	expression tag	UNP Q97W02
A	349	HIS	-	expression tag	UNP Q97W02

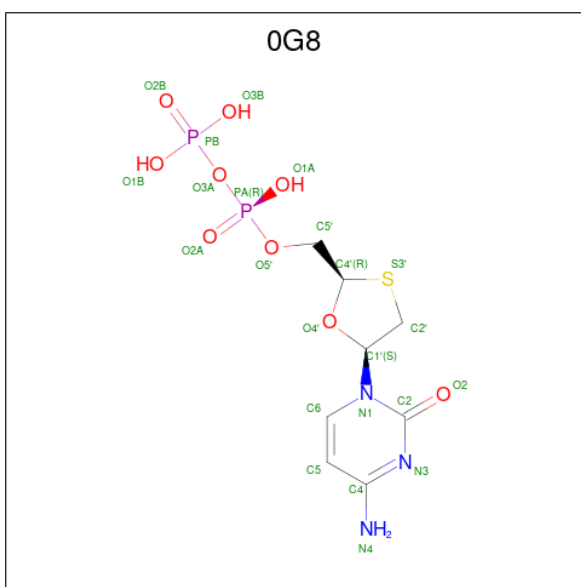
- Molecule 2 is a DNA chain called DNA (5'-D(P*GP*GP*CP*TP*AP*CP*AP*GP*GP*AP*CP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	13	Total	C	N	O	P	0	0	0
			264	126	51	75	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	16	Total	C	N	O	P	0	0	0
			329	155	61	97	16			

- Molecule 4 is [(2R,5S)-5-(4-amino-2-oxopyrimidin-1(2H)-yl)-1,3-oxathiolan-2-yl]methyl trihydrogen diphosphate (CCD ID: 0G8) (formula: C₈H₁₃N₃O₉P₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	0	0
			23	8	3	9	2	1		

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Ca	0	0
			3	3		

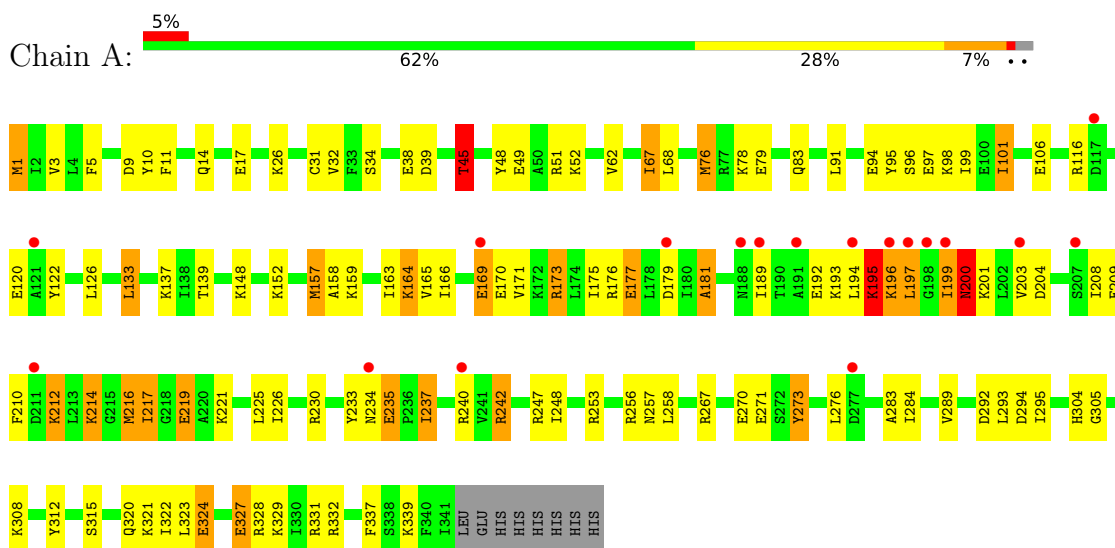
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	211	Total	O	0	0
			211	211		
6	C	31	Total	O	0	0
			31	31		
6	D	41	Total	O	0	0
			41	41		

3 Residue-property plots [i](#)

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

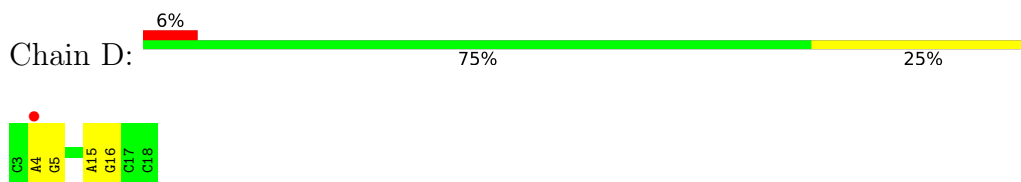
• Molecule 1: DNA polymerase IV



• Molecule 2: DNA (5'-D(P*GP*GP*CP*TP*AP*CP*AP*GP*GP*AP*CP*TP*C)-3')



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	96.18Å 102.64Å 52.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.20 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.3 (19.94-2.20) 96.1 (19.94-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.43 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.241 (Not available) , 0.291	Depositor DCC
R_{free} test set	4395 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3645	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% 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: CA, OG8

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	0.93	8/2782 (0.3%)	1.23	20/3736 (0.5%)
2	C	0.28	0/296	0.67	0/455
3	D	0.35	0/368	0.74	0/564
All	All	0.85	8/3446 (0.2%)	1.14	20/4755 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	ILE	CA-CB	-8.57	1.43	1.53
1	A	101	ILE	CA-CB	-6.91	1.45	1.53
1	A	216	MET	SD-CE	-6.74	1.62	1.79
1	A	1	MET	SD-CE	-6.33	1.63	1.79
1	A	163	ILE	CA-CB	-5.87	1.46	1.54
1	A	157	MET	SD-CE	-5.69	1.65	1.79
1	A	189	ILE	CA-CB	-5.61	1.46	1.54
1	A	200	ASN	CA-C	-5.35	1.45	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ILE	N-CA-C	8.72	121.27	112.90
1	A	200	ASN	N-CA-C	-7.73	103.18	114.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	GLU	N-CA-C	7.04	122.24	112.45
1	A	199	ILE	N-CA-C	-6.71	99.13	108.12
1	A	164	LYS	N-CA-C	6.52	119.11	108.55
1	A	11	PHE	N-CA-C	6.24	121.60	111.37
1	A	235	GLU	CA-C-N	6.00	125.76	119.76
1	A	235	GLU	C-N-CA	6.00	125.76	119.76
1	A	195	LYS	N-CA-C	-5.80	98.44	110.80
1	A	45	THR	CB-CA-C	-5.79	99.98	111.91
1	A	192	GLU	N-CA-C	-5.75	104.92	111.07
1	A	219	GLU	N-CA-C	5.64	117.11	111.07
1	A	31	CYS	N-CA-C	5.50	118.55	109.85
1	A	258	LEU	N-CA-C	5.50	117.72	111.11
1	A	237	ILE	N-CA-CB	-5.37	104.71	111.31
1	A	158	ALA	N-CA-C	5.33	120.44	113.30
1	A	181	ALA	N-CA-C	-5.32	106.30	112.89
1	A	67	ILE	N-CA-C	5.31	116.79	111.00
1	A	322	ILE	CB-CA-C	-5.20	105.32	111.97
1	A	217	ILE	CB-CA-C	-5.10	104.88	111.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	TYR	Sidechain

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	2743	0	2889	156	3
2	C	264	0	147	13	0
3	D	329	0	180	6	0
4	A	23	0	10	5	0
5	A	3	0	0	0	0
6	A	211	0	0	77	1
6	C	31	0	0	8	0
6	D	41	0	0	2	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3645	0	3226	174	3

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 26.

All (174) 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:A:196:LYS:O	1:A:197:LEU:HD23	1.36	1.20
1:A:176:ARG:HA	6:A:703:HOH:O	1.40	1.15
1:A:179:ASP:OD1	1:A:195:LYS:NZ	1.78	1.14
1:A:315:SER:HB3	6:A:695:HOH:O	1.54	1.05
1:A:175:ILE:HD11	6:A:575:HOH:O	1.60	1.00
1:A:197:LEU:HG	6:A:638:HOH:O	1.62	0.97
1:A:194:LEU:O	1:A:199:ILE:O	1.81	0.97
1:A:203:VAL:HB	6:A:703:HOH:O	1.62	0.96
1:A:193:LYS:HB3	1:A:216:MET:HE3	1.45	0.95
1:A:14:GLN:HE22	1:A:139:THR:H	1.14	0.94
1:A:196:LYS:C	1:A:197:LEU:HD23	1.97	0.89
1:A:199:ILE:HG13	6:A:708:HOH:O	1.72	0.89
1:A:157:MET:CE	1:A:164:LYS:HE3	2.02	0.88
1:A:45:THR:HG22	6:A:694:HOH:O	1.75	0.86
1:A:170:GLU:HB2	6:A:653:HOH:O	1.74	0.86
3:D:4:DA:H5''	3:D:4:DA:C8	2.11	0.85
1:A:171:VAL:CG1	6:A:575:HOH:O	2.24	0.85
1:A:196:LYS:O	1:A:196:LYS:HG3	1.76	0.84
1:A:193:LYS:O	1:A:196:LYS:HB3	1.76	0.84
1:A:248:ILE:HG23	6:D:140:HOH:O	1.77	0.83
1:A:171:VAL:HG12	6:A:575:HOH:O	1.79	0.83
1:A:284:ILE:HD11	6:A:695:HOH:O	1.78	0.82
1:A:45:THR:HG23	6:A:656:HOH:O	1.78	0.82
1:A:216:MET:SD	6:A:578:HOH:O	2.36	0.82
1:A:173:ARG:HD2	1:A:177:GLU:OE1	1.81	0.81
1:A:225:LEU:HD12	6:A:706:HOH:O	1.79	0.81
1:A:284:ILE:HD12	1:A:337:PHE:CE1	2.15	0.81
1:A:196:LYS:HD3	6:A:689:HOH:O	1.83	0.79
1:A:200:ASN:C	1:A:201:LYS:HG2	2.06	0.79
3:D:4:DA:C5'	3:D:4:DA:H8	1.96	0.79
1:A:284:ILE:CD1	6:A:695:HOH:O	2.31	0.77
1:A:116:ARG:HG3	1:A:120:GLU:OE2	1.85	0.77
3:D:4:DA:H5''	3:D:4:DA:H8	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:HE2	1:A:3:VAL:CG2	2.16	0.75
1:A:321:LYS:HD3	6:A:639:HOH:O	1.87	0.74
1:A:197:LEU:HG	6:A:708:HOH:O	1.88	0.74
1:A:230:ARG:NH2	6:A:672:HOH:O	2.21	0.73
1:A:193:LYS:HA	6:A:689:HOH:O	1.89	0.73
1:A:331:ARG:NH1	6:A:562:HOH:O	2.21	0.72
1:A:193:LYS:O	6:A:638:HOH:O	2.08	0.71
1:A:45:THR:HB	6:A:574:HOH:O	1.90	0.70
1:A:203:VAL:CB	6:A:703:HOH:O	2.28	0.70
1:A:176:ARG:HG2	6:A:703:HOH:O	1.92	0.70
1:A:194:LEU:O	1:A:199:ILE:HB	1.91	0.70
1:A:49:GLU:C	6:A:670:HOH:O	2.35	0.69
1:A:171:VAL:O	1:A:175:ILE:HG13	1.92	0.69
1:A:17:GLU:OE2	6:A:662:HOH:O	2.11	0.68
1:A:164:LYS:HG2	1:A:165:VAL:N	2.07	0.67
1:A:170:GLU:CB	6:A:653:HOH:O	2.35	0.67
1:A:199:ILE:CG1	6:A:708:HOH:O	2.36	0.67
1:A:52:LYS:HD2	6:A:676:HOH:O	1.95	0.67
1:A:14:GLN:NE2	1:A:139:THR:H	1.90	0.67
1:A:197:LEU:N	6:A:638:HOH:O	2.28	0.66
3:D:4:DA:C8	3:D:4:DA:C5'	2.75	0.66
1:A:51:ARG:NH2	4:A:401:OG8:O1A	2.29	0.65
1:A:214:LYS:O	1:A:214:LYS:HG3	1.96	0.65
1:A:292:ASP:O	1:A:293:LEU:HB2	1.97	0.65
1:A:78:LYS:HE2	6:A:634:HOH:O	1.95	0.64
1:A:157:MET:HE3	1:A:164:LYS:HE3	1.78	0.64
1:A:45:THR:HG21	4:A:401:OG8:O1A	1.98	0.64
1:A:235:GLU:N	6:A:655:HOH:O	2.30	0.63
2:C:4:DT:H2''	2:C:5:DA:H5'	1.80	0.63
1:A:48:TYR:O	1:A:52:LYS:HG3	1.99	0.62
1:A:304:HIS:HD2	1:A:305:GLY:O	1.83	0.62
1:A:52:LYS:HB2	6:A:670:HOH:O	2.00	0.62
1:A:78:LYS:HD2	6:A:657:HOH:O	1.99	0.62
2:C:12:DT:H1'	6:C:128:HOH:O	1.99	0.62
1:A:196:LYS:HB2	6:A:689:HOH:O	2.00	0.62
1:A:196:LYS:O	1:A:196:LYS:CG	2.48	0.61
1:A:289:VAL:HB	1:A:332:ARG:HB2	1.81	0.61
1:A:52:LYS:CB	6:A:670:HOH:O	2.48	0.61
1:A:157:MET:HE1	1:A:164:LYS:HE3	1.81	0.61
1:A:242:ARG:CD	6:A:692:HOH:O	2.50	0.59
1:A:203:VAL:CG1	6:A:703:HOH:O	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:DC:H5'	6:C:128:HOH:O	2.04	0.57
1:A:242:ARG:HD2	6:A:692:HOH:O	2.04	0.57
1:A:324:GLU:OE1	6:A:652:HOH:O	2.16	0.57
1:A:197:LEU:CG	6:A:708:HOH:O	2.49	0.57
1:A:233:TYR:OH	6:A:671:HOH:O	2.18	0.57
1:A:1:MET:N	6:A:701:HOH:O	2.37	0.56
1:A:45:THR:HG21	4:A:401:OG8:PA	2.46	0.56
2:C:13:DC:H5'	6:C:131:HOH:O	2.06	0.55
1:A:52:LYS:HG3	6:A:670:HOH:O	2.06	0.55
1:A:193:LYS:HB3	1:A:216:MET:CE	2.27	0.55
1:A:217:ILE:HD12	6:A:706:HOH:O	2.07	0.54
1:A:9:ASP:O	1:A:10:TYR:C	2.50	0.53
1:A:175:ILE:CD1	6:A:575:HOH:O	2.36	0.53
1:A:225:LEU:CD1	6:A:706:HOH:O	2.46	0.53
1:A:284:ILE:HD12	1:A:337:PHE:CZ	2.44	0.52
1:A:181:ALA:HB2	1:A:195:LYS:HE2	1.90	0.52
1:A:234:ASN:C	6:A:655:HOH:O	2.51	0.52
1:A:199:ILE:CD1	6:A:708:HOH:O	2.56	0.52
2:C:12:DT:C1'	6:C:128:HOH:O	2.55	0.52
1:A:1:MET:HE2	1:A:3:VAL:HG22	1.92	0.52
1:A:76:MET:HE1	6:D:102:HOH:O	2.10	0.51
1:A:214:LYS:HD2	1:A:219:GLU:HB2	1.92	0.51
1:A:78:LYS:CD	6:A:657:HOH:O	2.57	0.51
1:A:45:THR:HG21	4:A:401:OG8:O5'	2.11	0.51
1:A:49:GLU:O	6:A:670:HOH:O	2.18	0.51
1:A:194:LEU:HA	6:A:638:HOH:O	2.10	0.51
1:A:67:ILE:O	1:A:68:LEU:HD23	2.11	0.50
1:A:308:LYS:NZ	6:A:667:HOH:O	2.43	0.50
1:A:196:LYS:C	1:A:197:LEU:CD2	2.79	0.50
1:A:78:LYS:CE	6:A:634:HOH:O	2.57	0.49
3:D:15:DA:H2''	3:D:16:DG:OP2	2.12	0.49
1:A:176:ARG:CG	6:A:703:HOH:O	2.57	0.49
1:A:48:TYR:O	6:A:670:HOH:O	2.19	0.49
1:A:193:LYS:HD2	1:A:216:MET:HE3	1.95	0.49
1:A:52:LYS:CG	6:A:670:HOH:O	2.59	0.49
1:A:256:ARG:HG2	1:A:329:LYS:HG2	1.93	0.49
1:A:45:THR:CG2	6:A:656:HOH:O	2.51	0.48
1:A:152:LYS:CD	6:A:699:HOH:O	2.61	0.48
1:A:179:ASP:CG	1:A:195:LYS:NZ	2.63	0.48
1:A:97:GLU:HG2	1:A:98:LYS:HG3	1.96	0.47
1:A:217:ILE:CD1	6:A:706:HOH:O	2.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:9:DG:N7	6:C:119:HOH:O	2.36	0.47
1:A:176:ARG:O	1:A:201:LYS:HD2	2.14	0.47
2:C:4:DT:H2''	2:C:5:DA:C5'	2.45	0.47
2:C:13:DC:C5'	6:C:131:HOH:O	2.61	0.47
1:A:283:ALA:HB2	1:A:339:LYS:HD2	1.96	0.47
1:A:294:ASP:OD2	1:A:328:ARG:NH2	2.41	0.46
1:A:5:PHE:CE1	1:A:106:GLU:HB3	2.50	0.46
1:A:267:ARG:O	1:A:271:GLU:HG3	2.16	0.46
1:A:320:GLN:O	1:A:324:GLU:HB3	2.16	0.46
1:A:242:ARG:HD3	6:A:692:HOH:O	2.15	0.46
1:A:1:MET:CE	1:A:3:VAL:HG22	2.46	0.45
1:A:133:LEU:HD23	1:A:137:LYS:HA	1.99	0.45
1:A:193:LYS:C	1:A:196:LYS:HB3	2.41	0.45
1:A:166:ILE:HG23	1:A:170:GLU:HB3	1.98	0.45
1:A:170:GLU:OE2	1:A:173:ARG:NH2	2.50	0.45
1:A:91:LEU:O	1:A:94:GLU:HB3	2.16	0.45
1:A:95:TYR:O	1:A:96:SER:HB2	2.15	0.44
1:A:116:ARG:HA	6:A:615:HOH:O	2.17	0.44
1:A:52:LYS:N	6:A:670:HOH:O	2.44	0.44
1:A:10:TYR:HA	4:A:401:OG8:O1A	2.16	0.44
1:A:203:VAL:HG13	1:A:204:ASP:N	2.33	0.44
1:A:38:GLU:O	1:A:39:ASP:HB2	2.17	0.44
1:A:51:ARG:NH2	6:A:694:HOH:O	2.51	0.44
1:A:97:GLU:OE1	1:A:97:GLU:N	2.46	0.43
1:A:34:SER:HB3	3:D:5:DG:H5''	2.01	0.43
1:A:194:LEU:C	6:A:638:HOH:O	2.61	0.43
1:A:157:MET:HE3	1:A:164:LYS:CE	2.47	0.43
1:A:210:PHE:C	1:A:212:LYS:N	2.74	0.43
1:A:1:MET:HE3	1:A:237:ILE:HD12	2.00	0.42
1:A:203:VAL:HG11	6:A:703:HOH:O	2.15	0.42
1:A:208:ILE:HG12	1:A:209:GLU:N	2.33	0.42
2:C:5:DA:H5'	2:C:5:DA:C8	2.54	0.42
1:A:199:ILE:HD12	6:A:708:HOH:O	2.17	0.42
1:A:292:ASP:O	1:A:293:LEU:CB	2.62	0.42
2:C:10:DA:H8	6:C:127:HOH:O	2.01	0.42
2:C:13:DC:C4'	6:C:131:HOH:O	2.68	0.42
2:C:1:DG:H2''	2:C:2:DG:C8	2.53	0.42
2:C:3:DC:H2''	2:C:4:DT:H5'	2.02	0.42
1:A:1:MET:CB	6:A:701:HOH:O	2.67	0.42
1:A:26:LYS:HE3	6:A:687:HOH:O	2.20	0.42
1:A:273:TYR:HA	1:A:276:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HD3	1:A:237:ILE:HG12	2.00	0.41
1:A:221:LYS:NZ	6:A:508:HOH:O	2.53	0.41
1:A:1:MET:CE	1:A:3:VAL:CG2	2.95	0.41
1:A:226:ILE:CG2	6:A:672:HOH:O	2.67	0.41
1:A:32:VAL:HG22	1:A:76:MET:HE2	2.03	0.41
1:A:78:LYS:NZ	6:A:538:HOH:O	2.53	0.41
1:A:270:GLU:OE2	1:A:312:TYR:OH	2.32	0.41
1:A:193:LYS:HD2	1:A:216:MET:CE	2.51	0.41
1:A:122:TYR:CE2	1:A:126:LEU:HD11	2.56	0.41
1:A:152:LYS:HD2	6:A:699:HOH:O	2.21	0.41
1:A:315:SER:CB	6:A:695:HOH:O	2.36	0.41
1:A:101:ILE:O	1:A:240:ARG:HD2	2.20	0.41
1:A:159:LYS:HE2	1:A:159:LYS:HB3	1.86	0.40
1:A:181:ALA:HB2	1:A:195:LYS:CE	2.50	0.40
1:A:284:ILE:HD12	1:A:337:PHE:HE1	1.78	0.40
1:A:247:ARG:NH1	6:A:658:HOH:O	2.24	0.40
1:A:327:GLU:H	1:A:327:GLU:HG3	1.66	0.40
1:A:204:ASP:HB3	6:A:682:HOH:O	2.22	0.40

All (3) 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)
1:A:169:GLU:O	6:D:141:HOH:O[4_456]	1.64	0.56
1:A:173:ARG:N	6:D:141:HOH:O[4_456]	1.86	0.34
1:A:320:GLN:O	6:A:711:HOH:O[4_555]	2.18	0.02

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	339/349 (97%)	325 (96%)	14 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	300/308 (97%)	278 (93%)	22 (7%)	13	15

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	62	VAL
1	A	76	MET
1	A	79	GLU
1	A	83	GLN
1	A	99	ILE
1	A	133	LEU
1	A	169	GLU
1	A	173	ARG
1	A	195	LYS
1	A	196	LYS
1	A	197	LEU
1	A	200	ASN
1	A	212	LYS
1	A	214	LYS
1	A	242	ARG
1	A	253	ARG
1	A	257	ASN
1	A	295	ILE
1	A	323	LEU
1	A	324	GLU
1	A	327	GLU

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

Mol	Chain	Res	Type
1	A	14	GLN
1	A	130	ASN
1	A	188	ASN
1	A	200	ASN
1	A	285	HIS
1	A	304	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	OG8	A	401	5	23,24,24	1.01	0	33,36,36	1.10	3 (9%)

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
4	OG8	A	401	5	-	0/16/25/25	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	401	OG8	C4'-O4'-C1'	-2.98	106.55	112.68
4	A	401	OG8	C2'-S3'-C4'	2.51	94.64	88.41
4	A	401	OG8	C5-C6-N1	-2.17	118.30	121.84

There are no chirality outliers.

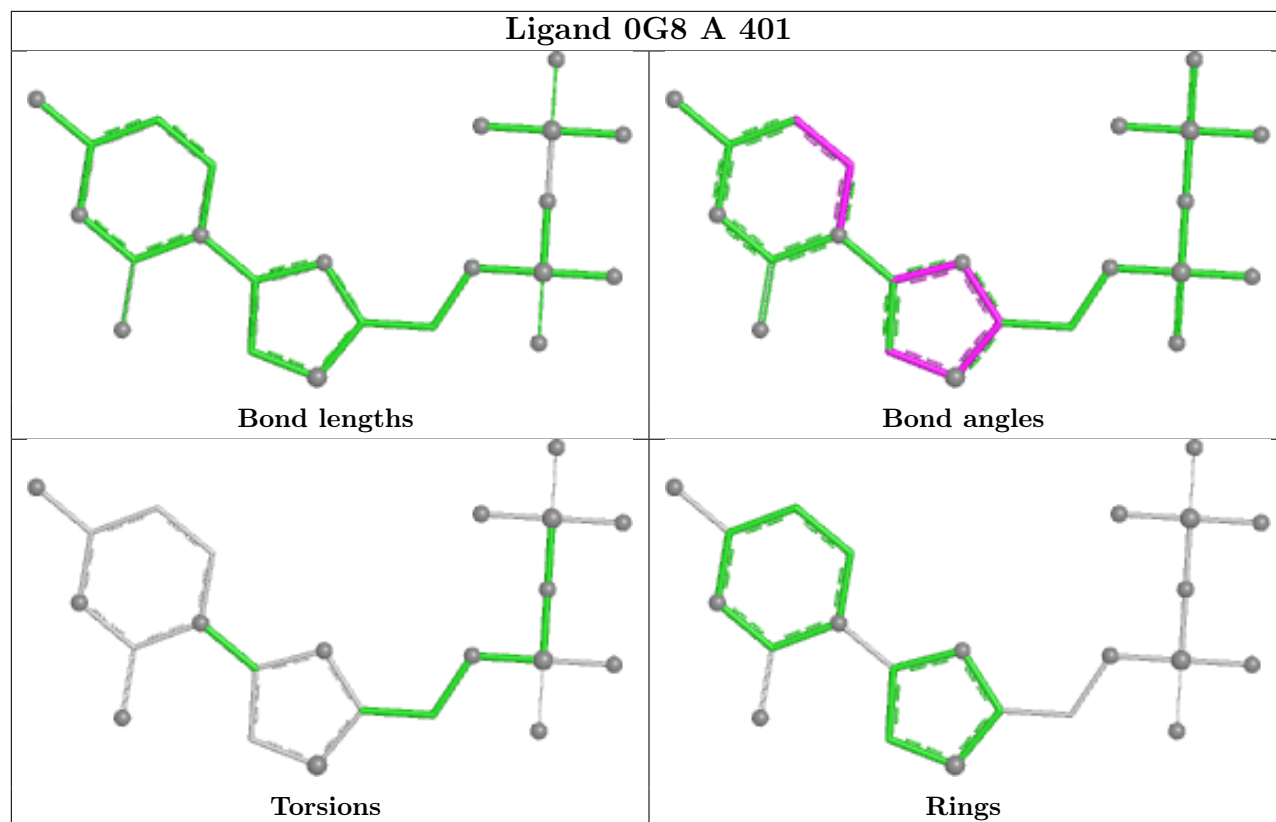
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	401	OG8	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	341/349 (97%)	0.42	18 (5%) 32 29	36, 56, 82, 95	0
2	C	13/13 (100%)	0.59	0 100 100	60, 65, 80, 84	0
3	D	16/16 (100%)	0.45	1 (6%) 26 23	50, 64, 106, 124	0
All	All	370/378 (97%)	0.43	19 (5%) 33 30	36, 57, 83, 124	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	198	GLY	5.3
1	A	197	LEU	4.0
1	A	179	ASP	3.2
1	A	194	LEU	3.1
1	A	211	ASP	2.7
1	A	169	GLU	2.5
1	A	196	LYS	2.4
1	A	277	ASP	2.3
1	A	240	ARG	2.3
1	A	203	VAL	2.3
1	A	207	SER	2.2
1	A	234	ASN	2.2
1	A	121	ALA	2.2
1	A	199	ILE	2.2
3	D	4	DA	2.2
1	A	191	ALA	2.2
1	A	188	ASN	2.1
1	A	117	ASP	2.1
1	A	189	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

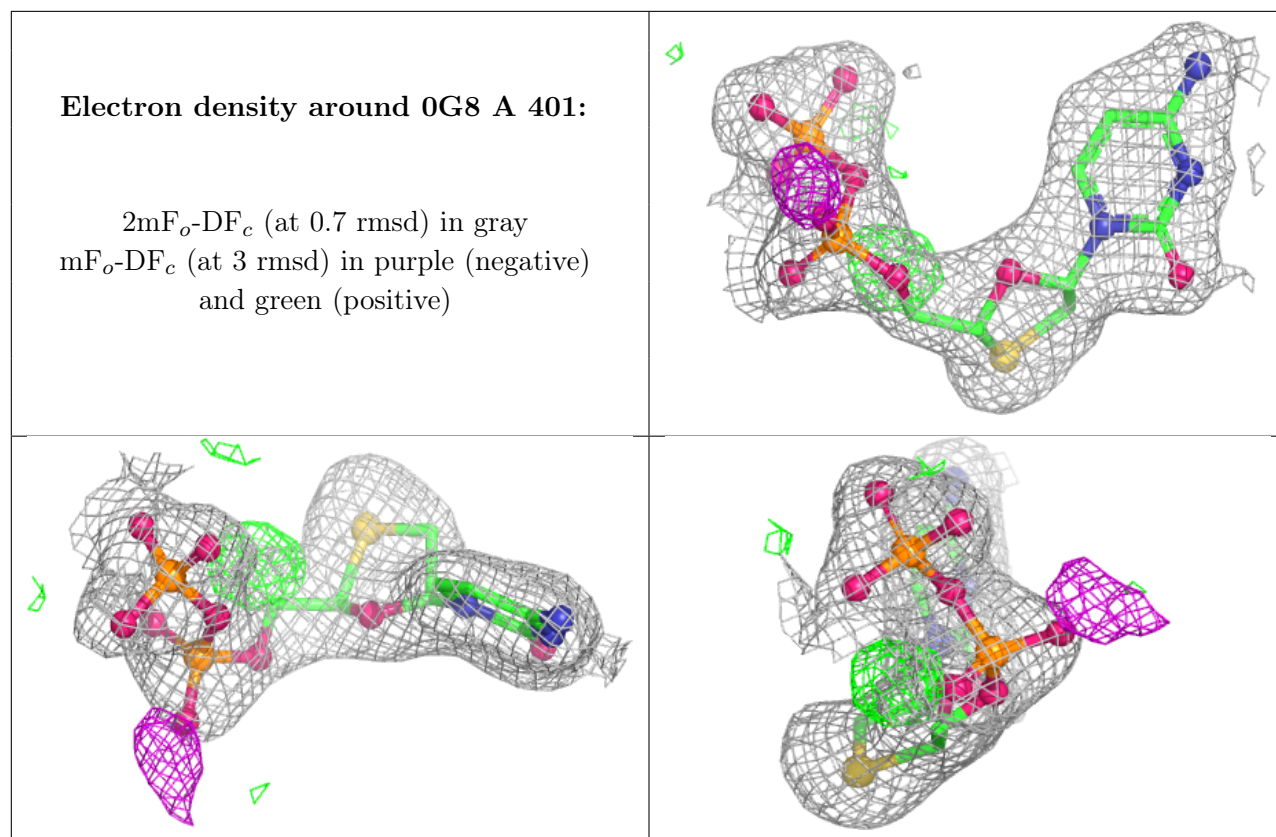
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
4	OG8	A	401	23/23	0.96	0.09	39,47,52,56	0
5	CA	A	402	1/1	0.98	0.04	52,52,52,52	0
5	CA	A	404	1/1	0.98	0.05	61,61,61,61	0
5	CA	A	403	1/1	0.99	0.02	41,41,41,41	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.