Full wwPDB X-ray Structure Validation Report ⓘ

Oct 29, 2026 – 12:09 pm GMT

PDB ID	:	31RF / pdb_000031rf
Title	:	POLQ-Taq chimera
Authors	:	Pflug, A.; Oliveira, T.M.
Deposited on	:	2026-06-18
Resolution	:	1.98 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:

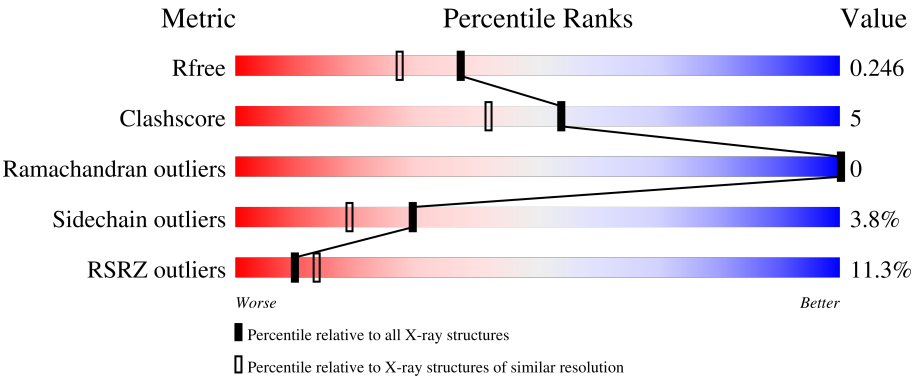
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.98 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.



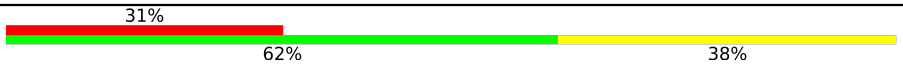
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	540	10% 87% 12%
1	D	540	13% 88% 11%
2	B	11	73% 27%
2	E	11	91% 9%
3	C	16	75% 25%

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Mol	Chain	Length	Quality of chain
3	F	16	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 10158 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 I, thermostable,DNA polymerase theta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	540	Total	C	N	O	S	0	3	0
			4259	2696	761	787	15			
1	D	540	Total	C	N	O	S	0	2	0
			4244	2687	756	786	15			

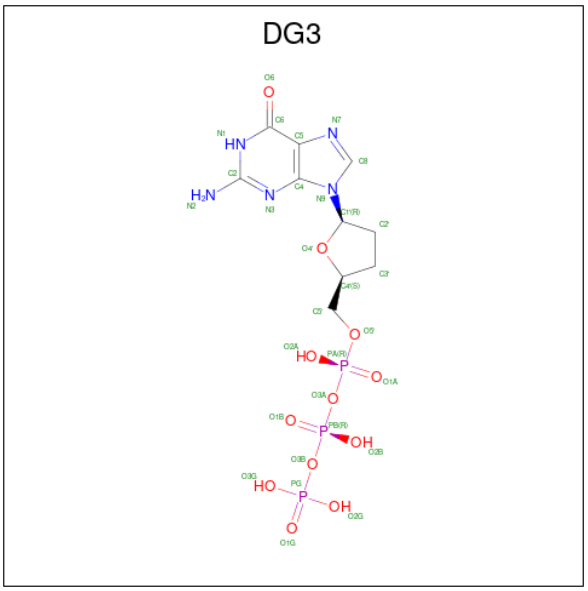
- Molecule 2 is a DNA chain called DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			
2	E	11	Total	C	N	O	P	0	0	0
			222	105	45	62	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	16	Total	C	N	O	P	0	0	0
			326	155	64	92	15			
3	F	16	Total	C	N	O	P	0	0	0
			326	155	64	92	15			

- Molecule 4 is 2'-3'-DIDEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DG3) (formula: $C_{10}H_{16}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O P 30 10 5 12 3	0	0
4	D	1	Total C N O P 30 10 5 12 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0

- Molecule 6 is water.

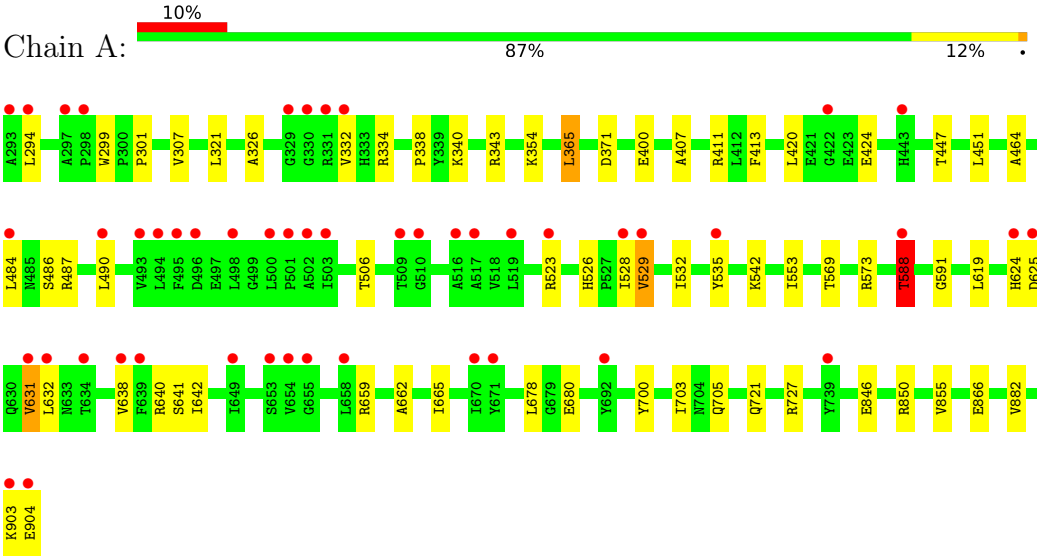
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	295	Total O 295 295	0	0
6	B	4	Total O 4 4	0	0
6	C	12	Total O 12 12	0	0
6	D	185	Total O 185 185	0	0
6	F	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

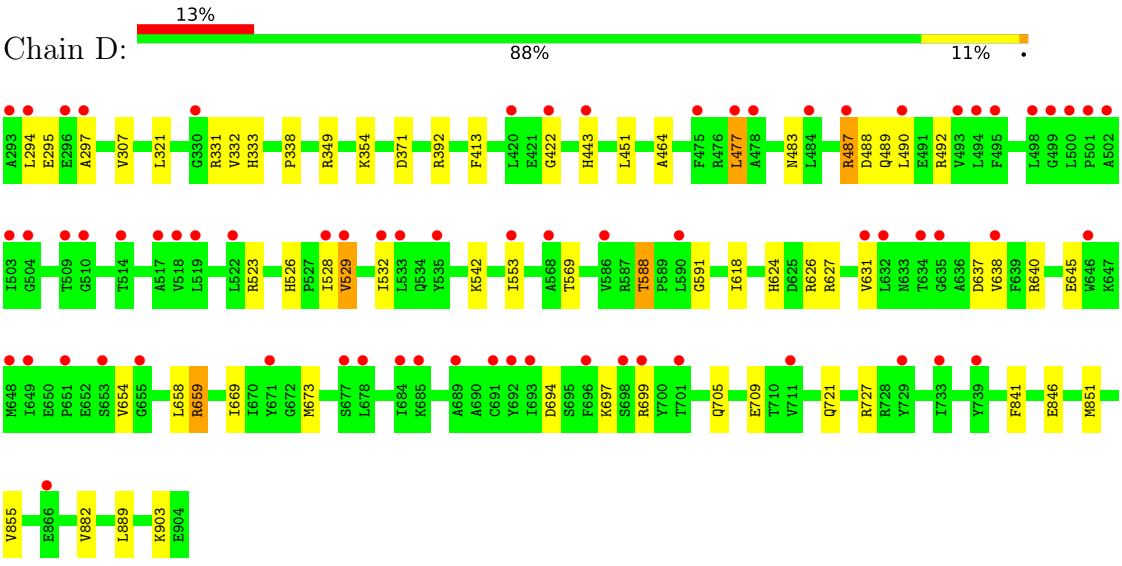
• Molecule 1: DNA polymerase I, thermostable,DNA polymerase theta

Chain A:



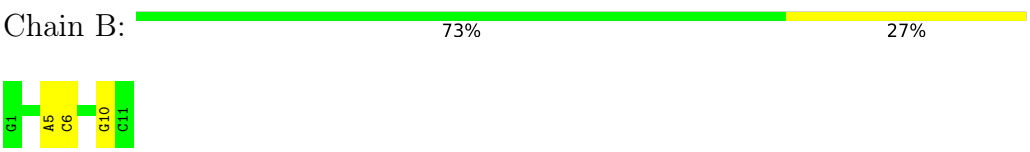
• Molecule 1: DNA polymerase I, thermostable,DNA polymerase theta

Chain D:



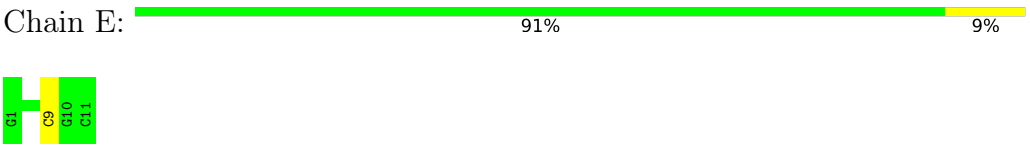
• Molecule 2: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*C)-3')

Chain B:



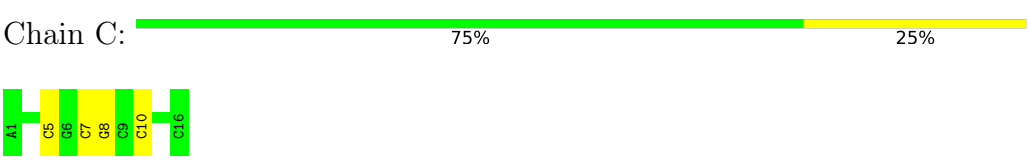
• Molecule 2: DNA (5'-D(*GP*AP*CP*CP*AP*CP*GP*GP*CP*GP*C)-3')

Chain E:



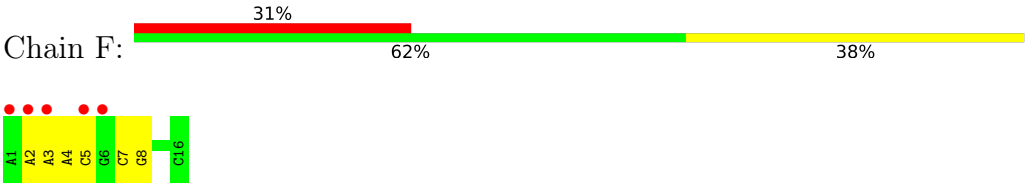
• Molecule 3: DNA (5'-D(*AP*AP*AP*AP*CP*GP*CP*GP*CP*CP*GP*TP*GP*GP*TP*C)-3')

Chain C:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.42Å 80.31Å 95.87Å 90.00° 93.96° 90.00°	Depositor
Resolution (Å)	61.51 – 1.98 61.51 – 1.98	Depositor EDS
% Data completeness (in resolution range)	99.5 (61.51-1.98) 99.5 (61.51-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 1.98Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.222 , 0.251 0.215 , 0.246	Depositor DCC
R_{free} test set	4469 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10158	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.69 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.1284e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DG3, MG

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	0.77	0/4342	1.07	5/5881 (0.1%)
1	D	0.70	1/4327 (0.0%)	1.05	5/5863 (0.1%)
2	B	0.80	0/249	0.76	0/382
2	E	0.81	0/249	0.81	0/382
3	C	0.89	0/366	0.76	0/563
3	F	0.91	0/366	0.77	0/563
All	All	0.75	1/9899 (0.0%)	1.02	10/13634 (0.1%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	618	ILE	CG1-CD1	-5.43	1.30	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	VAL	CA-C-N	8.81	127.64	121.65
1	A	307	VAL	C-N-CA	8.81	127.64	121.65
1	D	307	VAL	CA-C-N	8.30	127.29	121.65
1	D	307	VAL	C-N-CA	8.30	127.29	121.65
1	D	694	ASP	CA-C-N	5.80	128.06	120.28
1	D	694	ASP	C-N-CA	5.80	128.06	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	889	LEU	N-CA-C	-5.41	100.98	109.25
1	A	588	THR	CB-CA-C	5.37	116.93	108.88
1	A	640	ARG	N-CA-C	-5.21	105.51	111.14
1	D	889	LEU	N-CA-C	-5.18	101.33	109.25

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	299	TRP	Peptide

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	4259	0	4288	39	0
1	D	4244	0	4265	43	0
2	B	222	0	123	2	0
2	E	222	0	123	3	0
3	C	326	0	180	3	0
3	F	326	0	180	12	0
4	A	30	0	12	0	0
4	D	30	0	12	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	295	0	0	1	0
6	B	4	0	0	0	0
6	C	12	0	0	0	0
6	D	185	0	0	3	0
6	F	1	0	0	0	0
All	All	10158	0	9183	92	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 5.

All (92) 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:D:487:ARG:HD3	2:E:9:DC:H4'	1.42	0.97
1:D:721:GLN:NE2	1:D:727:ARG:HE	1.70	0.89
1:D:721:GLN:HE21	1:D:727:ARG:HE	1.22	0.88
1:D:487:ARG:CD	2:E:9:DC:H4'	2.06	0.85
1:A:721:GLN:NE2	1:A:727:ARG:HE	1.73	0.85
1:A:631:VAL:HG11	1:A:642:ILE:HG13	1.61	0.82
1:A:721:GLN:HE21	1:A:727:ARG:HE	1.28	0.81
1:A:424[A]:GLU:HG2	6:D:2750:HOH:O	1.81	0.80
1:D:297:ALA:HB3	1:D:333:HIS:CE1	2.20	0.76
1:A:588:THR:HG22	1:A:591:GLY:H	1.53	0.72
1:A:424[B]:GLU:OE2	1:D:624:HIS:NE2	2.23	0.70
1:A:627:ARG:HG2	1:A:700:TYR:CE1	2.25	0.70
1:D:673:MET:HG2	3:F:2:DA:OP1	1.92	0.70
1:D:443[B]:HIS:HE1	1:D:851:MET:H	1.40	0.69
1:D:588:THR:HG22	1:D:591:GLY:H	1.57	0.69
1:A:526:HIS:CD2	1:A:528:ILE:HG22	2.32	0.65
3:F:3:DA:H2'	3:F:4:DA:H1'	1.78	0.64
1:A:343:ARG:HA	1:A:365:LEU:HD21	1.78	0.64
1:D:721:GLN:HE22	1:D:727:ARG:HH21	1.48	0.62
1:D:443[B]:HIS:CE1	1:D:851:MET:H	2.17	0.62
1:A:490:LEU:HD11	1:A:532:ILE:HD13	1.80	0.62
1:D:526:HIS:CD2	1:D:528:ILE:HG22	2.35	0.61
3:F:3:DA:H2'	3:F:4:DA:C1'	2.30	0.61
1:A:631:VAL:HG13	1:A:641:SER:HB2	1.82	0.60
1:A:294:LEU:HD21	1:A:407:ALA:HB2	1.84	0.60
1:A:721:GLN:HE22	1:A:727:ARG:HH21	1.50	0.58
1:D:705:GLN:O	1:D:709:GLU:HG2	2.04	0.58
1:D:487:ARG:HD2	2:E:9:DC:O3'	2.04	0.57
3:F:3:DA:C2'	3:F:4:DA:H4'	2.36	0.56
1:A:332:VAL:HG11	1:A:334:ARG:NH1	2.22	0.55
3:F:3:DA:H2'	3:F:4:DA:C4'	2.38	0.54
3:F:3:DA:H2'	3:F:4:DA:H4'	1.90	0.53
1:D:297:ALA:CB	1:D:333:HIS:CE1	2.90	0.53
1:D:349:ARG:HD3	6:D:2726:HOH:O	2.08	0.52
1:D:295:GLU:HB3	1:D:331:ARG:HG2	1.92	0.51
1:A:477:LEU:HD23	1:A:528:ILE:HA	1.93	0.51
2:B:5:DA:H2"	2:B:6:DC:H5"	1.93	0.51
1:D:627:ARG:HH12	1:D:699:ARG:NH1	2.09	0.51
1:D:488:ASP:HB3	1:D:492:ARG:HH21	1.75	0.51
3:F:4:DA:C2	3:F:5:DC:N3	2.79	0.51
1:D:654:VAL:HG13	1:D:658:LEU:HD23	1.92	0.51
1:D:483:ASN:H	1:D:489:GLN:NE2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:ARG:HD2	1:D:371:ASP:HB2	1.92	0.50
3:F:4:DA:N3	3:F:5:DC:N3	2.59	0.50
1:A:573:ARG:HD3	6:A:2765:HOH:O	2.11	0.50
1:D:477:LEU:HD23	1:D:528:ILE:HA	1.93	0.49
1:D:294:LEU:HB2	1:D:332:VAL:CG1	2.43	0.49
1:A:625:ASP:OD2	1:A:628:LEU:HB2	2.12	0.49
1:A:301:PRO:HB3	1:A:326:ALA:HB3	1.95	0.48
1:D:443[B]:HIS:ND1	1:D:841:PHE:HE1	2.11	0.48
1:D:569:THR:HG22	3:F:5:DC:H4'	1.96	0.48
1:D:371:ASP:HB3	1:D:413:PHE:CE1	2.49	0.47
1:A:642:ILE:HG22	1:A:662:ALA:HB1	1.96	0.47
1:A:407:ALA:O	1:A:411:ARG:HD3	2.15	0.47
1:D:349:ARG:NH1	1:D:371:ASP:OD2	2.48	0.47
1:A:371:ASP:HB3	1:A:413:PHE:CE1	2.49	0.46
1:D:669:ILE:HD13	1:D:697:LYS:HG3	1.97	0.46
1:A:721:GLN:NE2	1:A:727:ARG:NE	2.55	0.46
1:D:631:VAL:HG22	1:D:645:GLU:HG3	1.98	0.45
1:A:294:LEU:HD22	1:A:332:VAL:HB	1.98	0.45
1:D:637:ASP:HB3	1:D:640:ARG:HB2	1.98	0.45
1:A:464:ALA:HB2	1:A:542:LYS:HE3	1.98	0.45
1:A:665:ILE:HD13	1:A:678:LEU:HD21	1.98	0.45
1:A:526:HIS:HD2	1:A:528:ILE:HG22	1.81	0.45
1:A:486:SER:HA	3:C:10:DC:H4'	1.97	0.44
1:D:483:ASN:H	1:D:489:GLN:HE22	1.65	0.44
1:A:451:LEU:HD12	1:A:553:ILE:HD11	2.00	0.44
1:A:506:THR:HG22	2:B:10:DG:OP2	2.17	0.44
1:D:451:LEU:HD12	1:D:553:ILE:HD11	1.99	0.44
1:A:526:HIS:HD2	1:A:528:ILE:H	1.66	0.44
1:A:619:LEU:HD21	1:A:703:ILE:HG12	2.00	0.43
1:D:464:ALA:HB2	1:D:542:LYS:HE3	2.01	0.43
1:A:321:LEU:HG	1:A:338:PRO:HB2	2.02	0.42
1:D:526:HIS:HD2	1:D:528:ILE:H	1.67	0.42
1:A:343:ARG:HG2	1:A:365:LEU:HD11	2.01	0.42
1:D:321:LEU:HG	1:D:338:PRO:HB2	2.02	0.42
1:A:569:THR:HA	3:C:5:DC:O5'	2.19	0.41
3:C:7:DC:H2'	3:C:8:DG:C8	2.55	0.41
1:D:490:LEU:HD11	1:D:532:ILE:HD13	2.02	0.41
1:D:721:GLN:NE2	1:D:727:ARG:NE	2.53	0.41
1:D:523:ARG:HA	1:D:529:VAL:HG22	2.03	0.41
1:A:484:LEU:HB3	1:A:535:TYR:CE2	2.55	0.41
1:D:659:ARG:HD2	6:D:2798:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ARG:HA	1:A:529:VAL:HG22	2.03	0.41
1:A:624:HIS:NE2	1:D:422:GLY:HA2	2.36	0.41
3:F:2:DA:H2"	3:F:3:DA:C8	2.55	0.41
1:D:526:HIS:CD2	1:D:528:ILE:CG2	3.04	0.40
1:A:632:LEU:HD23	1:A:887:VAL:HG21	2.03	0.40
1:A:447:THR:HG21	1:A:850:ARG:HD3	2.03	0.40
3:F:3:DA:H2'	3:F:4:DA:O4'	2.21	0.40
3:F:7:DC:H2'	3:F:8:DG:C8	2.57	0.40
1:D:297:ALA:HB3	1:D:333:HIS:ND1	2.35	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	541/540 (100%)	528 (98%)	13 (2%)	0	100	100
1	D	540/540 (100%)	526 (97%)	14 (3%)	0	100	100
All	All	1081/1080 (100%)	1054 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	439/441 (100%)	419 (95%)	20 (5%)	24 12
1	D	437/441 (99%)	424 (97%)	13 (3%)	36 27
All	All	876/882 (99%)	843 (96%)	33 (4%)	29 19

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	340	LYS
1	A	354	LYS
1	A	365	LEU
1	A	400	GLU
1	A	420	LEU
1	A	477	LEU
1	A	487	ARG
1	A	529	VAL
1	A	588	THR
1	A	631	VAL
1	A	638	VAL
1	A	659	ARG
1	A	680	GLU
1	A	705	GLN
1	A	846	GLU
1	A	855	VAL
1	A	866	GLU
1	A	882	VAL
1	A	903	LYS
1	A	904	GLU
1	D	354	LYS
1	D	392	ARG
1	D	477	LEU
1	D	487	ARG
1	D	529	VAL
1	D	588	THR
1	D	626	ARG
1	D	638	VAL
1	D	659	ARG
1	D	846	GLU
1	D	855	VAL
1	D	882	VAL
1	D	903	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	526	HIS
1	A	713	ASN
1	A	721	GLN
1	A	856	HIS
1	D	333	HIS
1	D	489	GLN
1	D	526	HIS
1	D	566	GLN
1	D	713	ASN
1	D	721	GLN
1	D	856	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, 2 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	$\#\|Z\| > 2$
4	DG3	A	2601	5	28,32,32	0.44	0	40,50,50	0.39	0
4	DG3	D	2601	5	28,32,32	0.53	0	40,50,50	0.42	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
4	DG3	A	2601	5	-	2/22/31/31	0/3/3/3
4	DG3	D	2601	5	-	2/22/31/31	0/3/3/3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

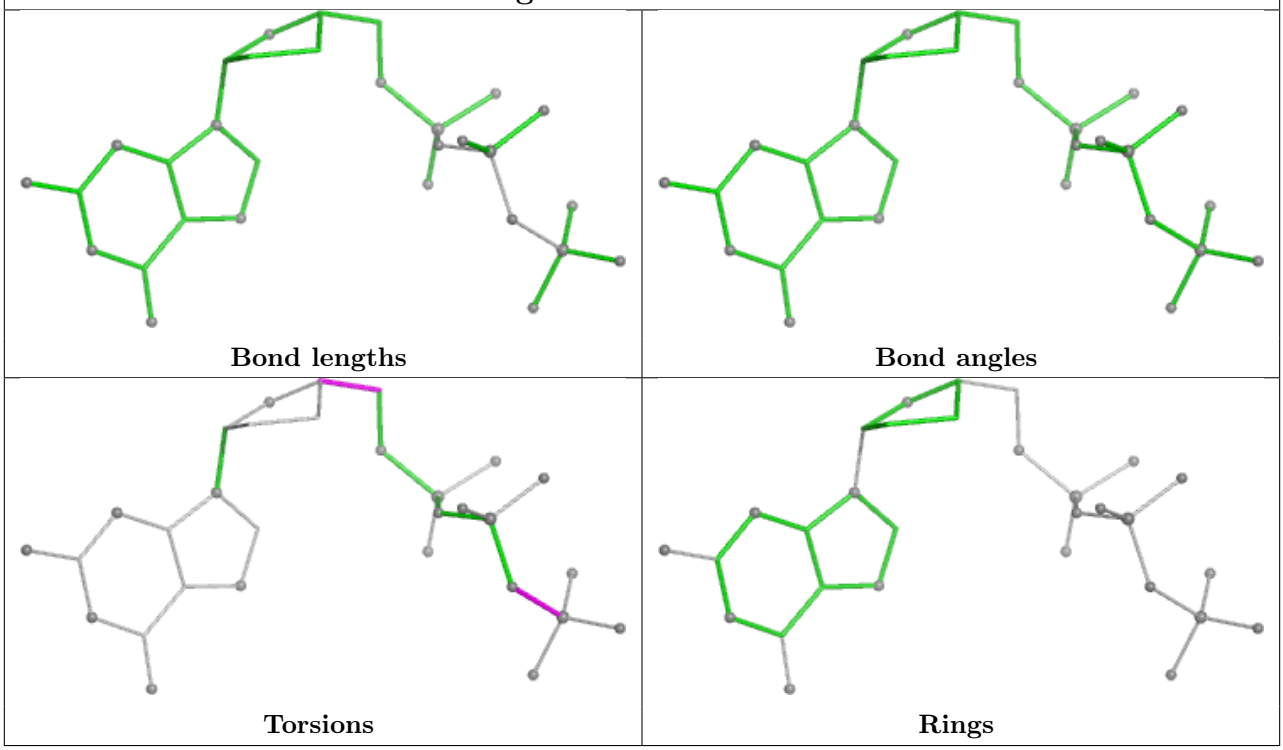
Mol	Chain	Res	Type	Atoms
4	A	2601	DG3	O4'-C4'-C5'-O5'
4	A	2601	DG3	PB-O3B-PG-O2G
4	D	2601	DG3	O4'-C4'-C5'-O5'
4	D	2601	DG3	PB-O3A-PA-O2A

There are no ring outliers.

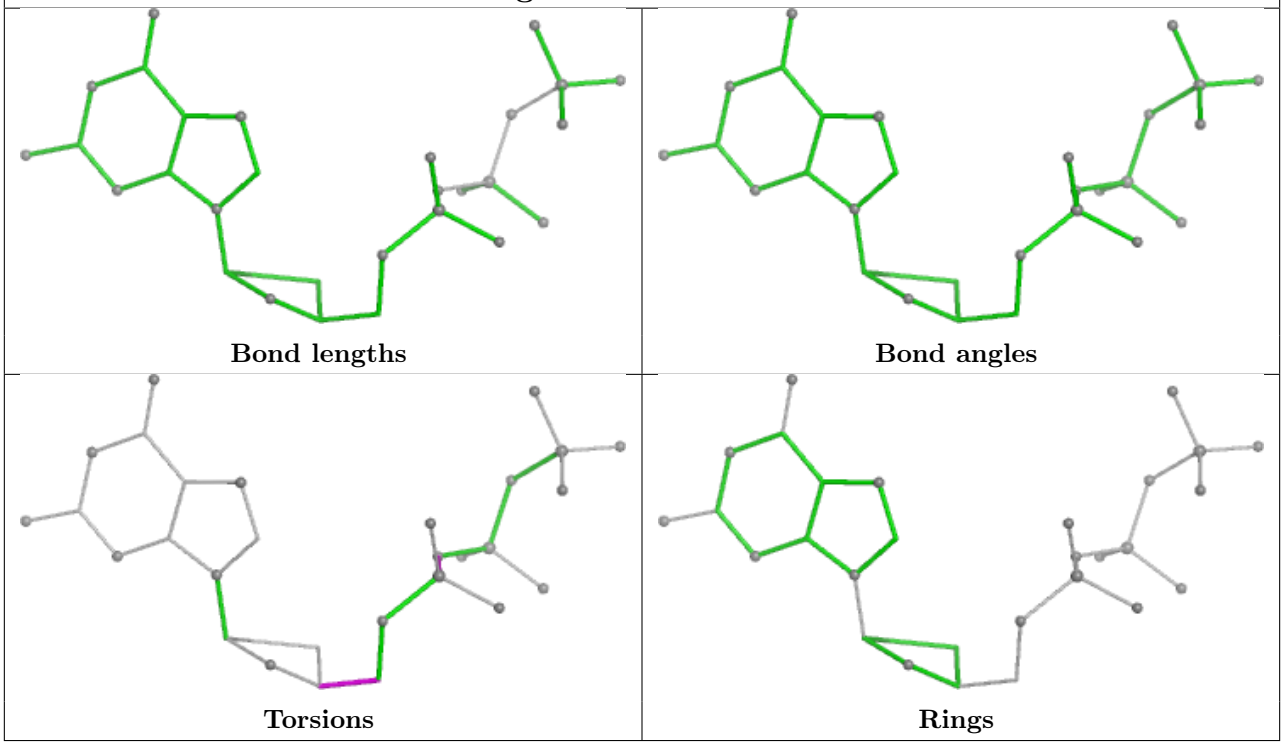
No monomer is involved in short contacts.

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

Ligand DG3 A 2601



Ligand DG3 D 2601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	540/540 (100%)	0.53	54 (10%) 12 18	14, 43, 92, 109	3 (0%)
1	D	540/540 (100%)	0.92	69 (12%) 7 11	20, 58, 105, 133	2 (0%)
2	B	11/11 (100%)	0.89	0 100 100	101, 121, 161, 165	0
2	E	11/11 (100%)	0.74	0 100 100	99, 125, 148, 153	0
3	C	16/16 (100%)	0.78	0 100 100	63, 94, 162, 193	0
3	F	16/16 (100%)	1.31	5 (31%) 1 1	90, 133, 172, 175	0
All	All	1134/1134 (100%)	0.74	128 (11%) 10 13	14, 53, 108, 193	5 (0%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ALA	6.5
1	D	493	VAL	6.0
1	A	503	ILE	5.7
1	D	503	ILE	5.5
1	D	499	GLY	5.4
1	A	293	ALA	4.9
1	A	628	LEU	4.9
1	D	495	PHE	4.7
1	D	510	GLY	4.7
1	D	501	PRO	4.6
1	D	500	LEU	4.6
1	A	294	LEU	4.5
1	A	502	ALA	4.4
1	D	696	PHE	4.2
1	D	692	TYR	4.1
1	A	477	LEU	4.0
1	A	490	LEU	3.9
1	D	671	TYR	3.9
1	D	519	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	494	LEU	3.7
1	D	498	LEU	3.7
1	D	293	ALA	3.7
1	D	689	ALA	3.7
1	A	498	LEU	3.6
1	D	490	LEU	3.6
1	A	654	VAL	3.6
1	A	494	LEU	3.6
1	A	638	VAL	3.5
1	D	294	LEU	3.5
1	A	655	GLY	3.5
1	A	500	LEU	3.5
1	D	649	ILE	3.5
1	D	698	SER	3.4
1	D	632	LEU	3.3
1	A	329	GLY	3.3
1	D	586	VAL	3.3
1	D	477	LEU	3.3
1	A	535	TYR	3.2
1	D	553	ILE	3.2
1	D	484	LEU	3.2
1	A	739	TYR	3.2
1	D	693	ILE	3.2
1	D	739	TYR	3.2
1	A	528	ILE	3.1
1	D	646	TRP	3.1
1	D	420	LEU	3.1
1	A	629	ILE	3.0
1	A	658	LEU	3.0
1	A	625	ASP	3.0
1	A	510	GLY	3.0
1	D	422	GLY	3.0
3	F	5	DC	2.9
1	D	504	GLY	2.9
1	D	518	VAL	2.8
1	D	517	ALA	2.8
1	A	519	LEU	2.8
1	A	523	ARG	2.8
1	D	733	ILE	2.8
1	D	509	THR	2.8
1	A	495	PHE	2.8
1	D	711	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	298	PRO	2.7
1	A	332	VAL	2.7
3	F	6	DG	2.7
1	D	635	GLY	2.7
1	D	684	ILE	2.7
1	D	866	GLU	2.6
1	A	632	LEU	2.6
1	D	528	ILE	2.6
1	D	478	ALA	2.6
1	D	487	ARG	2.6
1	D	296	GLU	2.6
1	A	624	HIS	2.5
1	D	729	TYR	2.5
1	A	904	GLU	2.5
1	A	484	LEU	2.5
1	A	649	ILE	2.5
1	D	638	VAL	2.5
1	D	699	ARG	2.5
1	D	648	MET	2.5
1	D	522	LEU	2.5
1	D	678	LEU	2.5
1	A	422	GLY	2.5
1	A	330	GLY	2.5
3	F	1	DA	2.5
1	A	653	SER	2.5
1	D	677	SER	2.5
1	A	588	THR	2.5
1	A	470	LEU	2.4
1	D	634	THR	2.4
1	A	493	VAL	2.4
1	D	443[A]	HIS	2.4
1	D	297	ALA	2.4
1	A	671	TYR	2.4
1	A	297	ALA	2.4
1	A	516	ALA	2.4
1	D	568	ALA	2.4
1	D	653	SER	2.4
1	A	639	PHE	2.3
1	D	685	LYS	2.3
1	D	651	PRO	2.3
1	D	655	GLY	2.3
1	A	627	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	533	LEU	2.3
1	D	590	LEU	2.3
1	A	903	LYS	2.3
1	D	532	ILE	2.3
1	D	514	THR	2.3
3	F	2	DA	2.3
1	D	330	GLY	2.2
1	A	634	THR	2.2
1	D	701	THR	2.2
1	A	331	ARG	2.2
1	A	631	VAL	2.2
1	A	501	PRO	2.2
1	D	529	VAL	2.2
1	A	517	ALA	2.2
1	D	535	TYR	2.1
1	A	529	VAL	2.1
1	A	496	ASP	2.1
1	D	631	VAL	2.1
1	D	691	CYS	2.1
1	D	475	PHE	2.1
1	A	509	THR	2.1
1	A	443[A]	HIS	2.1
1	A	670	ILE	2.0
1	A	692	TYR	2.0
3	F	3	DA	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

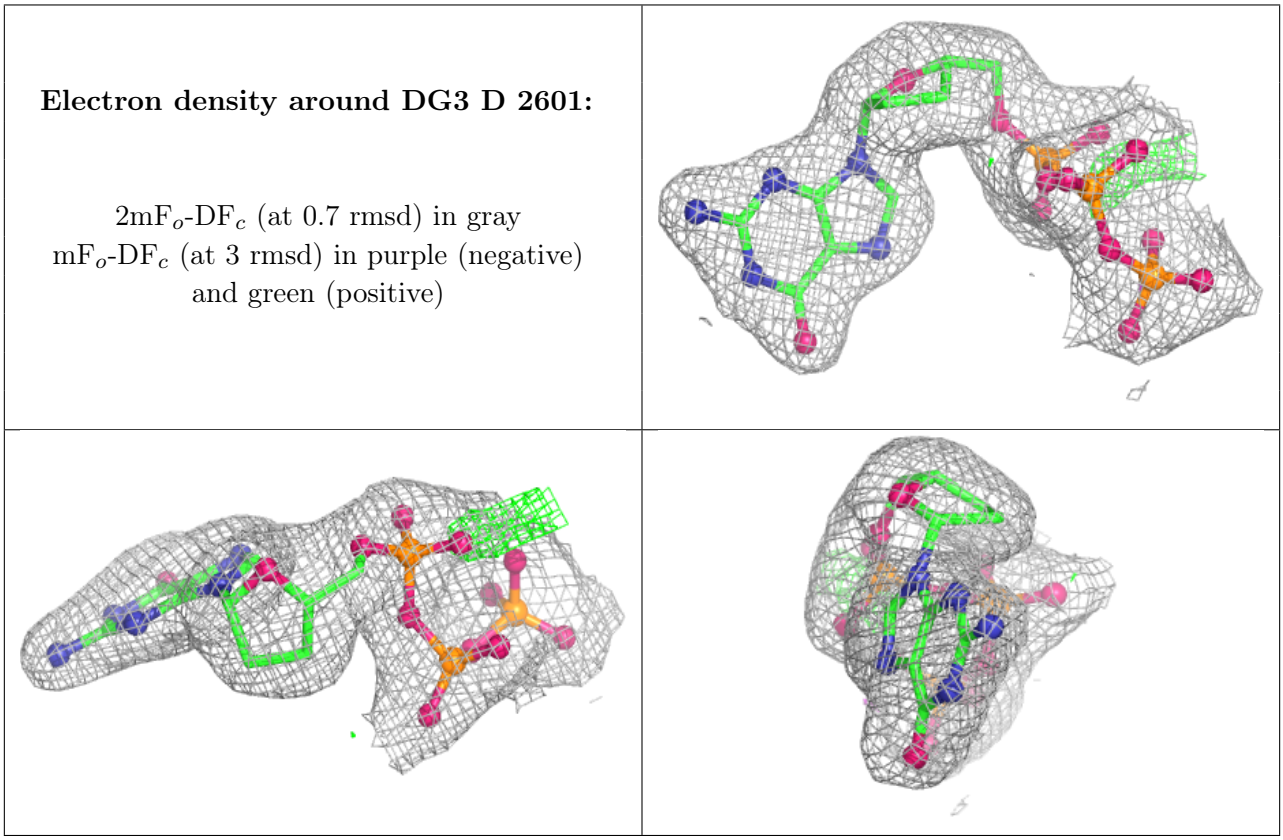
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	MG	D	2602	1/1	0.95	0.10	44,44,44,44	0
5	MG	A	2602	1/1	0.96	0.09	44,44,44,44	0
4	DG3	D	2601	30/30	0.96	0.07	38,42,45,45	0
4	DG3	A	2601	30/30	0.98	0.05	35,38,39,40	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.

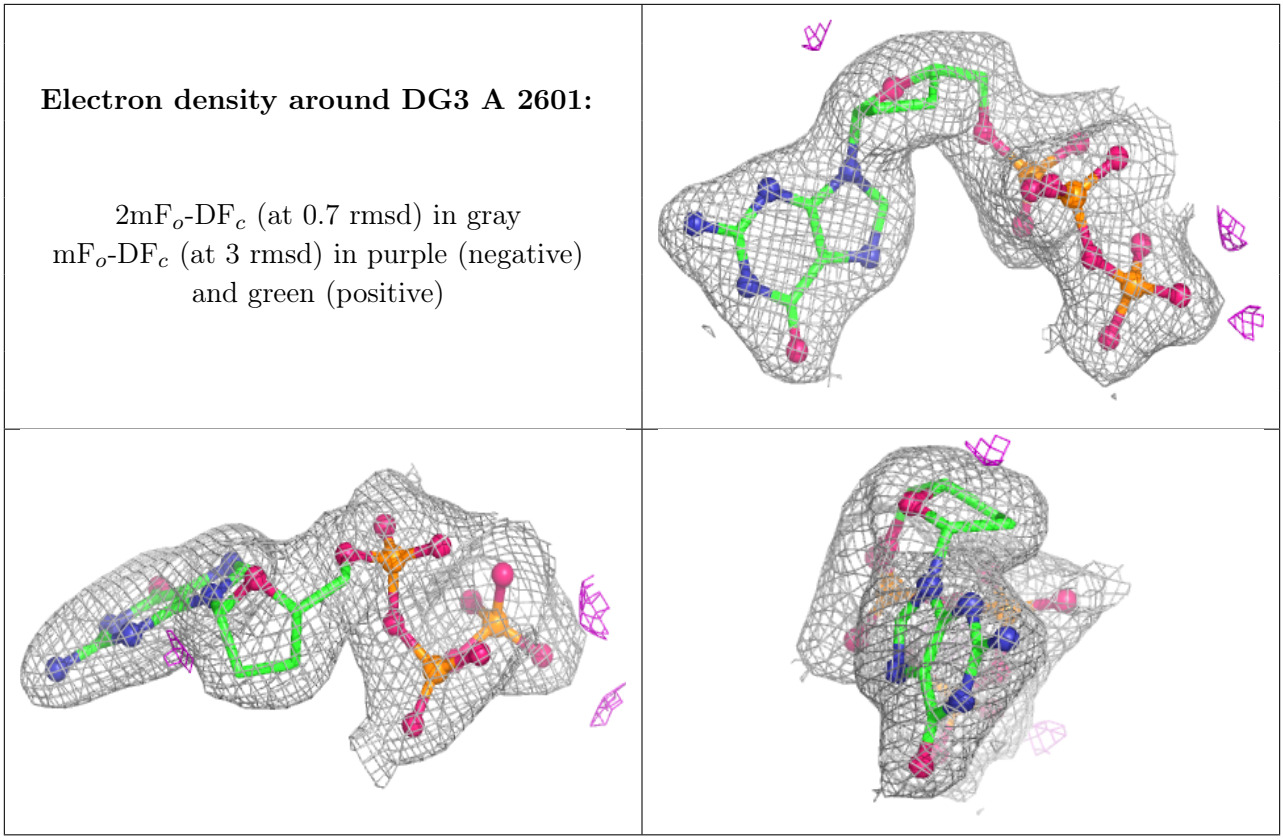
Electron density around DG3 D 2601:

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



Electron density around DG3 A 2601:

$2mF_o$-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.