



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:01 AM UTC

PDB ID : 6CST / pdb_00006cst
Title : Structure of human DNA polymerase kappa with DNA
Authors : Jha, V.; Ling, H.
Deposited on : 2018-03-21
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

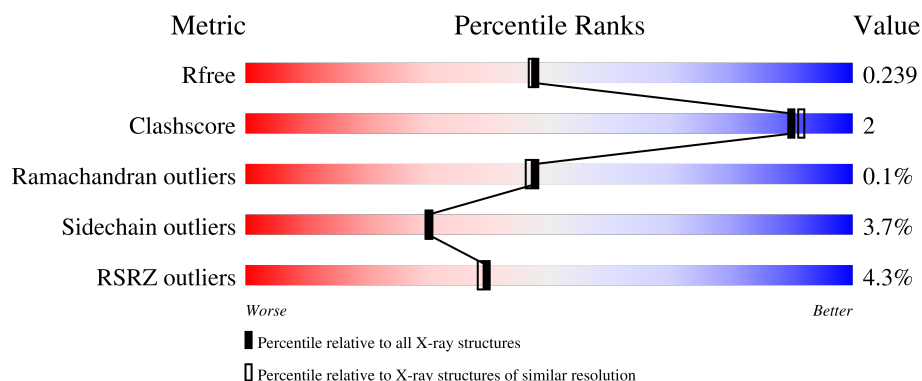
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	551	3% 74% 7% 19%
1	B	551	4% 75% 5% 20%
2	C	9	89% 11%
2	P	9	89% 11%
3	D	13	77% 23%

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Mol	Chain	Length	Quality of chain
3	T	13	 77%23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	603	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 8536 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 kappa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3517	2219	623	653	22			
1	B	442	Total	C	N	O	S	0	1	0
			3470	2189	612	647	22			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	initiating methionine	UNP Q9UBT6
A	-23	SER	-	expression tag	UNP Q9UBT6
A	-22	TYR	-	expression tag	UNP Q9UBT6
A	-21	TYR	-	expression tag	UNP Q9UBT6
A	-20	HIS	-	expression tag	UNP Q9UBT6
A	-19	HIS	-	expression tag	UNP Q9UBT6
A	-18	HIS	-	expression tag	UNP Q9UBT6
A	-17	HIS	-	expression tag	UNP Q9UBT6
A	-16	HIS	-	expression tag	UNP Q9UBT6
A	-15	HIS	-	expression tag	UNP Q9UBT6
A	-14	ASP	-	expression tag	UNP Q9UBT6
A	-13	TYR	-	expression tag	UNP Q9UBT6
A	-12	ASP	-	expression tag	UNP Q9UBT6
A	-11	ILE	-	expression tag	UNP Q9UBT6
A	-10	PRO	-	expression tag	UNP Q9UBT6
A	-9	THR	-	expression tag	UNP Q9UBT6
A	-8	THR	-	expression tag	UNP Q9UBT6
A	-7	GLU	-	expression tag	UNP Q9UBT6
A	-6	ASN	-	expression tag	UNP Q9UBT6
A	-5	LEU	-	expression tag	UNP Q9UBT6
A	-4	TYR	-	expression tag	UNP Q9UBT6
A	-3	PHE	-	expression tag	UNP Q9UBT6
A	-2	GLN	-	expression tag	UNP Q9UBT6
A	-1	GLY	-	expression tag	UNP Q9UBT6
A	0	ALA	-	expression tag	UNP Q9UBT6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-24	MET	-	initiating methionine	UNP Q9UBT6
B	-23	SER	-	expression tag	UNP Q9UBT6
B	-22	TYR	-	expression tag	UNP Q9UBT6
B	-21	TYR	-	expression tag	UNP Q9UBT6
B	-20	HIS	-	expression tag	UNP Q9UBT6
B	-19	HIS	-	expression tag	UNP Q9UBT6
B	-18	HIS	-	expression tag	UNP Q9UBT6
B	-17	HIS	-	expression tag	UNP Q9UBT6
B	-16	HIS	-	expression tag	UNP Q9UBT6
B	-15	HIS	-	expression tag	UNP Q9UBT6
B	-14	ASP	-	expression tag	UNP Q9UBT6
B	-13	TYR	-	expression tag	UNP Q9UBT6
B	-12	ASP	-	expression tag	UNP Q9UBT6
B	-11	ILE	-	expression tag	UNP Q9UBT6
B	-10	PRO	-	expression tag	UNP Q9UBT6
B	-9	THR	-	expression tag	UNP Q9UBT6
B	-8	THR	-	expression tag	UNP Q9UBT6
B	-7	GLU	-	expression tag	UNP Q9UBT6
B	-6	ASN	-	expression tag	UNP Q9UBT6
B	-5	LEU	-	expression tag	UNP Q9UBT6
B	-4	TYR	-	expression tag	UNP Q9UBT6
B	-3	PHE	-	expression tag	UNP Q9UBT6
B	-2	GLN	-	expression tag	UNP Q9UBT6
B	-1	GLY	-	expression tag	UNP Q9UBT6
B	0	ALA	-	expression tag	UNP Q9UBT6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			181	87	33	52	9			
2	P	9	Total	C	N	O	P	0	0	0
			181	87	33	52	9			

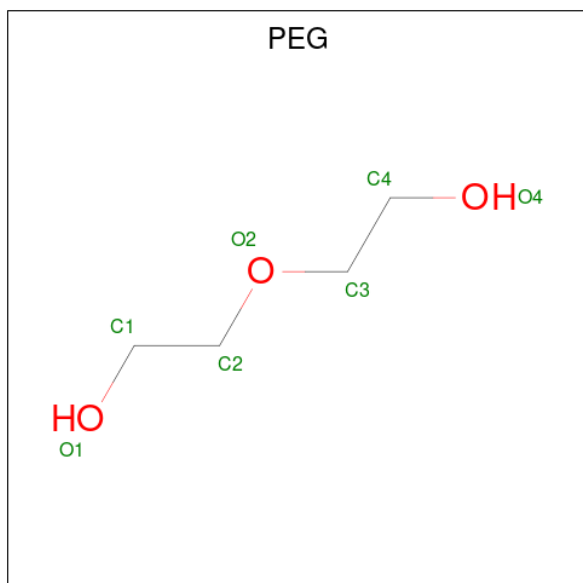
- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*AP*CP*TP*GP*GP*TP*AP*TP*GP*TP*AP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			268	129	45	81	13			
3	T	13	Total	C	N	O	P	0	0	0
			268	129	45	81	13			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mg	0	0
			2	2		
4	B	2	Total	Mg	0	0
			2	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is IODIDE ION (CCD ID: IOD) (formula: I).

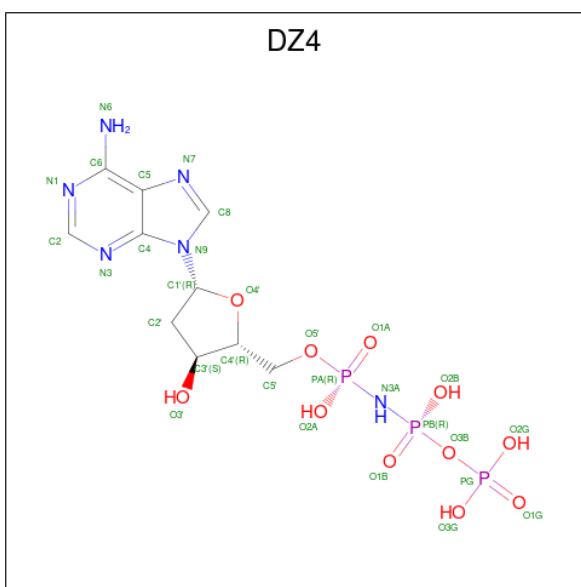
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total	I	0	0
			3	3		
6	B	3	Total	I	0	0
			3	3		

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



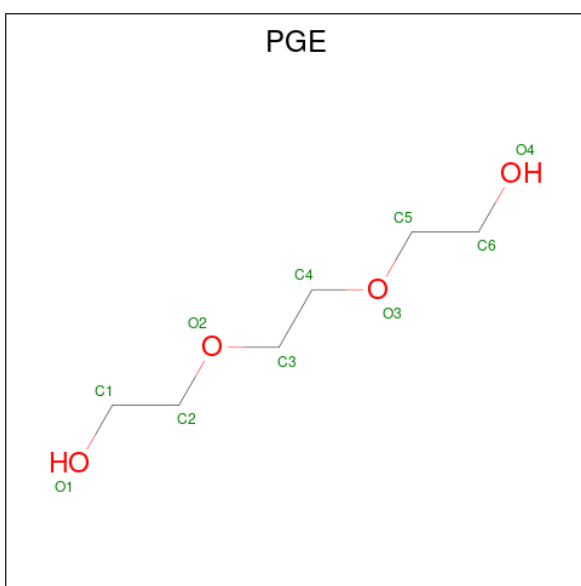
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is 2'-deoxy-5'-O-[(R)-hydroxy{[(R)-hydroxy(phosphonooxy)phosphoryl]amino}p
hosphoryl]adenosine (CCD ID: DZ4) (formula: $C_{10}H_{17}N_6O_{11}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	0
			30	10	6	11	3		
8	B	1	Total	C	N	O	P	0	0
			30	10	6	11	3		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	5	Total Cl 5 5	0	0
10	B	4	Total Cl 4 4	0	0

- Molecule 11 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	1	Total K 1 1	0	0
11	B	2	Total K 2 2	0	0
11	D	1	Total K 1 1	0	0

- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	243	Total O 243 243	0	0
12	B	173	Total O 173 173	0	0
12	C	17	Total O 17 17	0	0
12	D	18	Total O 18 18	0	0
12	P	12	Total O 12 12	0	0
12	T	20	Total O 20 20	0	0

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- Molecule 1: DNA polymerase kappa





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

Chain P:  89% 11%



- Molecule 3: DNA (5'-D(P*TP*AP*CP*TP*GP*GP*TP*AP*TP*GP*TP*AP*T)-3')

Chain D:  77% 23%



- Molecule 3: DNA (5'-D(P*TP*AP*CP*TP*GP*GP*TP*AP*TP*GP*TP*AP*T)-3')

Chain T:  77% 23%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	67.58Å 124.63Å 165.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.14 – 2.00 44.14 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (44.14-2.00) 98.1 (44.14-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.198 , 0.234 0.204 , 0.239	Depositor DCC
R_{free} test set	2327 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.868	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8536	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: PGE, K, IOD, DZ4, CL, PEG, MG, EDO

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	0.89	3/3570 (0.1%)	0.99	7/4803 (0.1%)
1	B	0.79	0/3526	0.94	3/4749 (0.1%)
2	C	0.43	0/202	0.98	0/308
2	P	0.38	0/202	0.91	0/308
3	D	0.43	0/299	1.11	3/460 (0.7%)
3	T	0.39	0/299	1.03	1/460 (0.2%)
All	All	0.80	3/8098 (0.0%)	0.97	14/11088 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	168	PRO	C-O	-7.27	1.18	1.25
1	A	167	VAL	C-N	5.78	1.38	1.33
1	A	167	VAL	C-O	-5.23	1.18	1.24

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	LYS	N-CA-C	6.65	119.38	111.33
1	B	123	LEU	N-CA-C	6.11	120.81	113.23
1	A	168	PRO	CA-C-O	-5.77	116.75	120.90
1	A	167	VAL	CA-C-N	-5.73	115.47	119.66
1	A	167	VAL	C-N-CA	-5.73	115.47	119.66
1	A	371	ILE	CB-CA-C	-5.72	105.31	110.91
1	A	291	GLN	CB-CG-CD	5.66	122.22	112.60
1	B	124	LYS	N-CA-C	5.57	118.88	111.75
1	B	506	LEU	N-CA-C	5.31	118.72	110.17
3	D	4	DC	C4'-C3'-O3'	-5.29	102.06	110.00
3	D	13	DA	C2'-C3'-O3'	5.14	119.22	111.50
3	D	4	DC	N1-C1'-C2'	5.09	121.13	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	LYS	N-CA-C	5.09	116.51	111.07
3	T	13	DA	C2'-C3'-O3'	5.05	119.08	111.50

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	3517	0	3564	20	0
1	B	3470	0	3487	8	0
2	C	181	0	102	0	2
2	P	181	0	102	0	1
3	D	268	0	150	0	1
3	T	268	0	150	1	2
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	28	0	40	5	0
5	B	7	0	10	1	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	36	0	54	1	0
7	B	4	0	6	1	0
8	A	30	0	13	0	0
8	B	30	0	13	0	0
9	A	10	0	14	0	0
10	A	5	0	0	0	0
10	B	4	0	0	0	0
11	A	1	0	0	0	0
11	B	2	0	0	0	0
11	D	1	0	0	0	0
12	A	243	0	0	2	0
12	B	173	0	0	0	0
12	C	17	0	0	0	0
12	D	18	0	0	0	0
12	P	12	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	T	20	0	0	0	0
All	All	8536	0	7705	29	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 2.

All (29) 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:141:TYR:H	5:A:603:PEG:H21	1.47	0.79
1:A:220:ARG:HD3	1:A:283:SER:OG	1.94	0.67
1:A:117:MET:HB3	1:A:124:LYS:HE2	1.76	0.65
1:A:436:GLN:NE2	12:A:706:HOH:O	2.37	0.50
1:B:377:TYR:HB2	1:B:399:SER:HB2	1.94	0.49
1:A:19:MET:CE	1:A:44:THR:HG21	2.43	0.49
1:A:220:ARG:CD	1:A:283:SER:OG	2.59	0.49
1:A:461:LYS:HB3	1:A:508:LEU:HB3	1.94	0.48
1:A:110:ALA:HB3	5:A:603:PEG:H31	1.95	0.48
1:B:141:TYR:HB2	5:B:603:PEG:H11	1.95	0.48
1:A:397:HIS:CG	5:A:604:PEG:H21	2.50	0.47
1:B:193:MET:HE3	1:B:407:LEU:HB3	1.97	0.46
1:A:141:TYR:HB2	5:A:603:PEG:H21	1.97	0.46
1:A:117:MET:HE2	1:A:124:LYS:HE2	1.98	0.46
1:B:429:GLU:HA	7:B:607:EDO:H22	1.97	0.46
1:A:19:MET:HE1	1:A:44:THR:HG21	1.98	0.45
1:B:44:THR:HG22	1:B:50:TYR:HB2	1.97	0.45
1:A:508:LEU:C	1:A:508:LEU:HD23	2.42	0.44
1:A:193:MET:HE3	1:A:407:LEU:HB3	1.99	0.44
1:A:44:THR:O	1:A:44:THR:HG22	2.17	0.44
1:B:394:TYR:CZ	1:B:398:ILE:HD11	2.53	0.43
1:A:195:MET:HB2	1:A:199:GLU:HG3	2.00	0.42
1:A:343:MET:HE1	1:A:400:LEU:O	2.19	0.42
1:A:446:LEU:HD11	1:A:513:ILE:HG21	2.02	0.42
1:A:141:TYR:HB2	5:A:603:PEG:C2	2.50	0.41
1:A:384:SER:HA	1:A:392:TRP:CD1	2.56	0.40
1:B:124:LYS:HB2	1:B:124:LYS:HE3	1.51	0.40
7:A:618:EDO:H21	12:A:819:HOH:O	2.21	0.40
1:B:44:THR:HG23	3:T:4:DC:N4	2.36	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)
3:D:14:DT:O3'	2:P:5:DA:P[3_657]	1.67	0.53
2:C:5:DA:P	3:T:14:DT:O3'[3_657]	2.04	0.16
2:C:5:DA:OP1	3:T:14:DT:O3'[3_657]	2.15	0.05

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	442/551 (80%)	432 (98%)	9 (2%)	1 (0%)	43	42
1	B	439/551 (80%)	426 (97%)	13 (3%)	0	100	100
All	All	881/1102 (80%)	858 (97%)	22 (2%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LEU

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	380/495 (77%)	366 (96%)	14 (4%)	30	30
1	B	372/495 (75%)	358 (96%)	14 (4%)	29	29
All	All	752/990 (76%)	724 (96%)	28 (4%)	30	30

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	LYS
1	A	42	GLU
1	A	48	ARG
1	A	65	GLU
1	A	70	GLN
1	A	73	GLN
1	A	88	ARG
1	A	122	GLU
1	A	124	LYS
1	A	148	VAL
1	A	158	LYS
1	A	198	ASP
1	A	325	ASP
1	A	434	LEU
1	B	29	GLU
1	B	122	GLU
1	B	124	LYS
1	B	128	ILE
1	B	158	LYS
1	B	163	GLN
1	B	198	ASP
1	B	306	THR
1	B	325	ASP
1	B	347	LYS
1	B	434	LEU
1	B	436	GLN
1	B	474	VAL
1	B	475	SER

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	83	GLN
1	A	212	GLN
1	B	66	ASN
1	B	77	GLN
1	B	163	GLN
1	B	340	GLN

5.3.3 RNA ⓘ

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 41 ligands modelled in this entry, 23 are monoatomic - leaving 18 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	$\# Z > 2$
5	PEG	A	603	-	6,6,6	0.44	0	5,5,5	0.31	0
7	EDO	A	618	-	3,3,3	0.43	0	2,2,2	0.49	0
7	EDO	A	610	-	3,3,3	0.62	0	2,2,2	0.29	0
7	EDO	A	615	-	3,3,3	0.57	0	2,2,2	0.25	0
5	PEG	B	603	-	6,6,6	0.66	0	5,5,5	0.59	0
7	EDO	A	617	-	3,3,3	0.41	0	2,2,2	0.90	0
9	PGE	A	620	-	9,9,9	0.45	0	8,8,8	0.42	0
5	PEG	A	604	-	6,6,6	0.44	0	5,5,5	0.30	0
5	PEG	A	606	-	6,6,6	0.65	0	5,5,5	0.58	0
5	PEG	A	605	-	6,6,6	0.54	0	5,5,5	0.33	0
7	EDO	A	611	-	3,3,3	0.38	0	2,2,2	0.40	0
7	EDO	A	612	-	3,3,3	0.30	0	2,2,2	0.33	0
7	EDO	A	613	-	3,3,3	0.50	0	2,2,2	0.21	0
7	EDO	A	614	-	3,3,3	0.51	0	2,2,2	0.36	0
7	EDO	A	616	-	3,3,3	0.25	0	2,2,2	0.31	0
8	DZ4	A	619	4	31,32,32	0.69	0	44,50,50	0.69	0
8	DZ4	B	608	4	31,32,32	0.71	0	44,50,50	0.81	1 (2%)
7	EDO	B	607	-	3,3,3	0.34	0	2,2,2	0.51	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
5	PEG	A	603	-	-	2/4/4/4	-
7	EDO	A	618	-	-	1/1/1/1	-
7	EDO	A	610	-	-	1/1/1/1	-
7	EDO	A	615	-	-	1/1/1/1	-
5	PEG	B	603	-	-	2/4/4/4	-
7	EDO	A	617	-	-	1/1/1/1	-
9	PGE	A	620	-	-	4/7/7/7	-
5	PEG	A	604	-	-	1/4/4/4	-
5	PEG	A	606	-	-	1/4/4/4	-
5	PEG	A	605	-	-	3/4/4/4	-
7	EDO	A	611	-	-	1/1/1/1	-
7	EDO	A	612	-	-	1/1/1/1	-
7	EDO	A	613	-	-	0/1/1/1	-
7	EDO	A	614	-	-	1/1/1/1	-
7	EDO	A	616	-	-	1/1/1/1	-
8	DZ4	A	619	4	-	7/19/34/34	0/3/3/3
8	DZ4	B	608	4	-	5/19/34/34	0/3/3/3
7	EDO	B	607	-	-	0/1/1/1	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	608	DZ4	C4-C5-N7	-2.11	108.17	110.58

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	619	DZ4	PB-N3A-PA-O5'
8	A	619	DZ4	PB-O3B-PG-O2G
8	B	608	DZ4	PB-O3B-PG-O2G
5	A	605	PEG	O1-C1-C2-O2
5	A	605	PEG	O2-C3-C4-O4
5	A	606	PEG	O2-C3-C4-O4
5	B	603	PEG	O1-C1-C2-O2
5	A	603	PEG	O1-C1-C2-O2
9	A	620	PGE	O3-C5-C6-O4
7	A	616	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
7	A	610	EDO	O1-C1-C2-O2
5	B	603	PEG	O2-C3-C4-O4
7	A	617	EDO	O1-C1-C2-O2
9	A	620	PGE	O2-C3-C4-O3
5	A	605	PEG	C4-C3-O2-C2
9	A	620	PGE	C1-C2-O2-C3
7	A	614	EDO	O1-C1-C2-O2
5	A	603	PEG	O2-C3-C4-O4
8	A	619	DZ4	PB-O3B-PG-O1G
8	B	608	DZ4	PB-O3B-PG-O1G
8	B	608	DZ4	PB-N3A-PA-O5'
7	A	611	EDO	O1-C1-C2-O2
5	A	604	PEG	O2-C3-C4-O4
7	A	612	EDO	O1-C1-C2-O2
8	A	619	DZ4	PB-N3A-PA-O1A
7	A	615	EDO	O1-C1-C2-O2
7	A	618	EDO	O1-C1-C2-O2
8	A	619	DZ4	PB-O3B-PG-O3G
8	B	608	DZ4	PB-O3B-PG-O3G
8	B	608	DZ4	C5'-O5'-PA-O1A
9	A	620	PGE	C6-C5-O3-C4
8	A	619	DZ4	C2'-C1'-N9-C4
8	A	619	DZ4	O4'-C1'-N9-C4

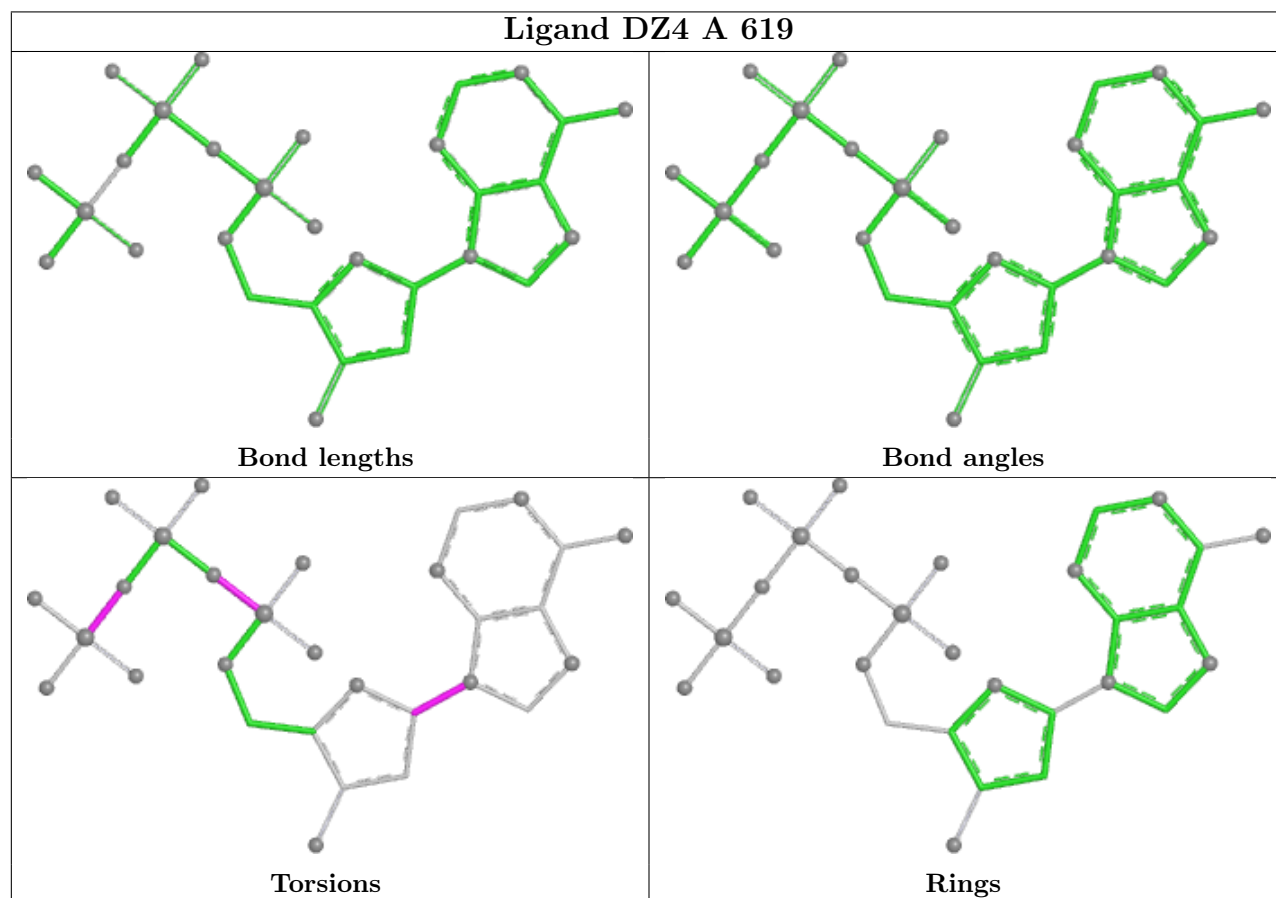
There are no ring outliers.

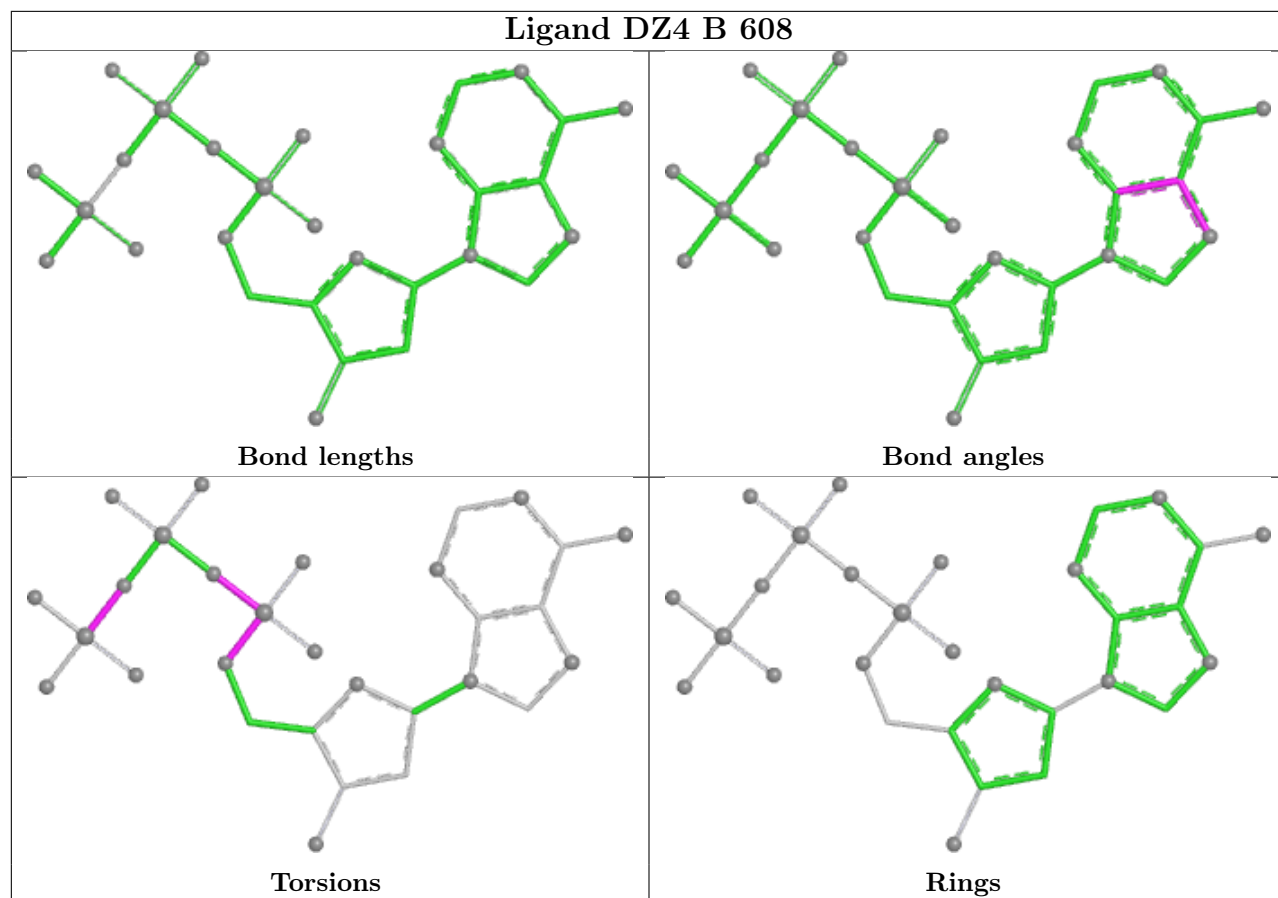
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	603	PEG	4	0
7	A	618	EDO	1	0
5	B	603	PEG	1	0
5	A	604	PEG	1	0
7	B	607	EDO	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	446/551 (80%)	0.16	17 (3%)	44	43	21, 34, 65, 104	0
1	B	442/551 (80%)	0.44	23 (5%)	33	31	25, 43, 76, 106	1 (0%)
2	C	9/9 (100%)	-0.31	0	100	100	30, 36, 48, 53	0
2	P	9/9 (100%)	-0.36	0	100	100	33, 36, 52, 52	0
3	D	13/13 (100%)	-0.23	0	100	100	27, 41, 48, 51	0
3	T	13/13 (100%)	-0.03	0	100	100	31, 45, 54, 54	0
All	All	932/1146 (81%)	0.27	40 (4%)	40	39	21, 40, 74, 106	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	5.3
1	A	410	ASP	5.2
1	B	26	ALA	5.0
1	A	282	ASN	4.5
1	B	31	LEU	4.4
1	B	22	ASN	4.3
1	A	18	ARG	4.2
1	B	518	ASN	4.2
1	A	20	GLY	4.1
1	A	222	PHE	4.1
1	A	19	MET	3.9
1	B	27	GLY	3.7
1	A	223	ILE	3.5
1	A	17	LEU	3.4
1	B	282	ASN	3.3
1	B	21	LEU	3.2
1	A	500	PHE	3.2
1	B	222	PHE	3.2
1	A	518	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	GLY	2.9
1	B	223	ILE	2.8
1	B	28	MET	2.7
1	B	448	LYS	2.7
1	B	20	GLY	2.6
1	B	412	GLU	2.5
1	A	474	VAL	2.5
1	B	346	ILE	2.5
1	A	73	GLN	2.5
1	B	25	LYS	2.4
1	B	30	GLY	2.4
1	B	410	ASP	2.3
1	B	500	PHE	2.3
1	A	408	THR	2.2
1	A	406	HIS	2.2
1	B	409	ARG	2.2
1	A	477	VAL	2.2
1	B	29	GLU	2.2
1	B	406	HIS	2.2
1	B	171	PHE	2.1
1	B	89	PHE	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
7	EDO	A	614	4/4	0.83	0.12	59,59,59,63	0
7	EDO	A	617	4/4	0.84	0.18	43,44,49,56	0

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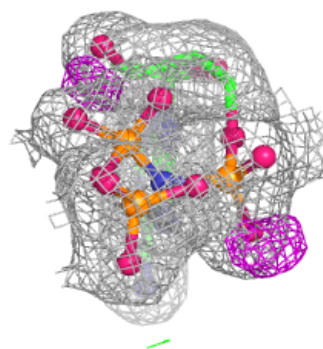
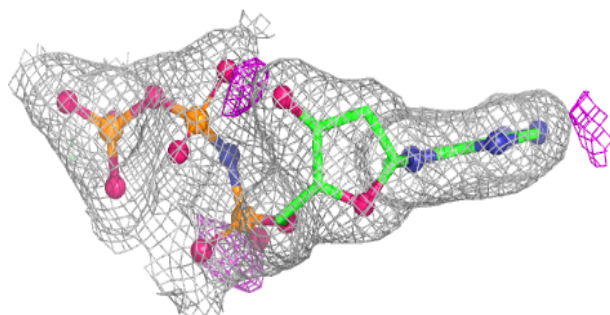
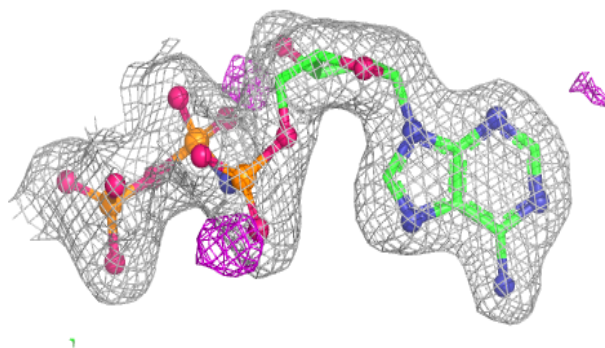
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	EDO	A	618	4/4	0.84	0.24	40,41,49,51	0
7	EDO	A	616	4/4	0.87	0.14	50,55,55,58	0
5	PEG	A	606	7/7	0.88	0.12	65,66,68,69	0
7	EDO	A	615	4/4	0.89	0.17	51,52,53,59	0
5	PEG	A	605	7/7	0.89	0.12	53,57,64,66	0
5	PEG	A	603	7/7	0.90	0.14	16,24,27,28	0
7	EDO	A	613	4/4	0.91	0.10	59,61,62,62	0
7	EDO	A	611	4/4	0.91	0.11	54,54,55,58	0
9	PGE	A	620	10/10	0.91	0.14	60,63,65,66	0
7	EDO	A	610	4/4	0.92	0.12	29,31,36,39	0
5	PEG	B	603	7/7	0.93	0.12	22,35,39,40	0
4	MG	B	602	1/1	0.94	0.08	55,55,55,55	0
4	MG	A	602	1/1	0.94	0.08	42,42,42,42	0
5	PEG	A	604	7/7	0.94	0.12	31,37,48,52	0
7	EDO	A	612	4/4	0.95	0.10	31,32,33,38	0
6	IOD	B	605	1/1	0.95	0.17	56,56,56,56	0
10	CL	A	621	1/1	0.96	0.11	53,53,53,53	0
10	CL	A	624	1/1	0.96	0.08	50,50,50,50	0
6	IOD	B	606	1/1	0.97	0.28	67,67,67,67	0
7	EDO	B	607	4/4	0.97	0.13	26,30,33,36	0
8	DZ4	B	608	30/30	0.97	0.06	25,30,33,34	0
10	CL	B	611	1/1	0.97	0.06	45,45,45,45	0
10	CL	B	612	1/1	0.97	0.08	59,59,59,59	0
10	CL	B	609	1/1	0.98	0.08	39,39,39,39	0
10	CL	B	610	1/1	0.98	0.07	54,54,54,54	0
6	IOD	A	609	1/1	0.98	0.17	68,68,68,68	0
8	DZ4	A	619	30/30	0.98	0.05	19,23,24,24	0
11	K	B	614	1/1	0.98	0.04	39,39,39,39	0
4	MG	B	601	1/1	0.99	0.08	28,28,28,28	0
10	CL	A	625	1/1	0.99	0.11	23,23,23,23	0
6	IOD	A	607	1/1	0.99	0.02	30,30,30,30	0
4	MG	A	601	1/1	0.99	0.07	19,19,19,19	0
6	IOD	B	604	1/1	0.99	0.14	64,64,64,64	0
10	CL	A	622	1/1	0.99	0.06	28,28,28,28	0
11	K	A	626	1/1	0.99	0.06	34,34,34,34	0
10	CL	A	623	1/1	0.99	0.09	23,23,23,23	0
11	K	D	101	1/1	0.99	0.06	34,34,34,34	0
6	IOD	A	608	1/1	1.00	0.08	37,37,37,37	0
11	K	B	613	1/1	1.00	0.01	29,29,29,29	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.

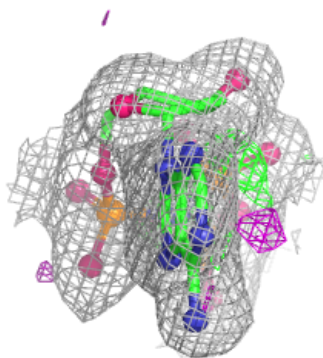
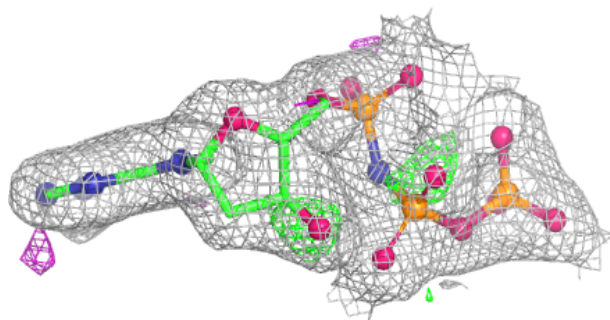
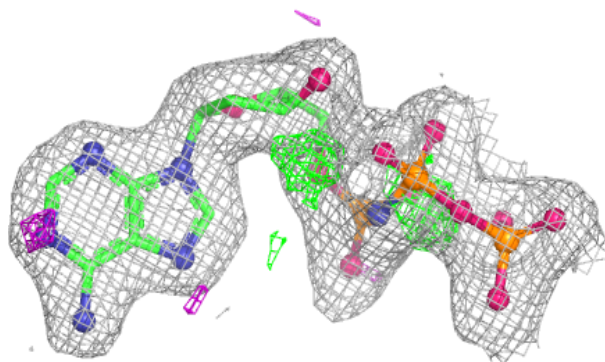
Electron density around DZ4 B 608:

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



Electron density around DZ4 A 619:

$2mF_o-DF_c$ (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.