



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:48 AM UTC

PDB ID : 2OZS / pdb_00002ozs
Title : Crystal structure of RB69 gp43 in complex with DNA with dATP opposite dTMP
Authors : Zahn, K.E.; Belrhali, H.; Wallace, S.S.; Doublié, S.
Deposited on : 2007-02-27
Resolution : 2.75 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

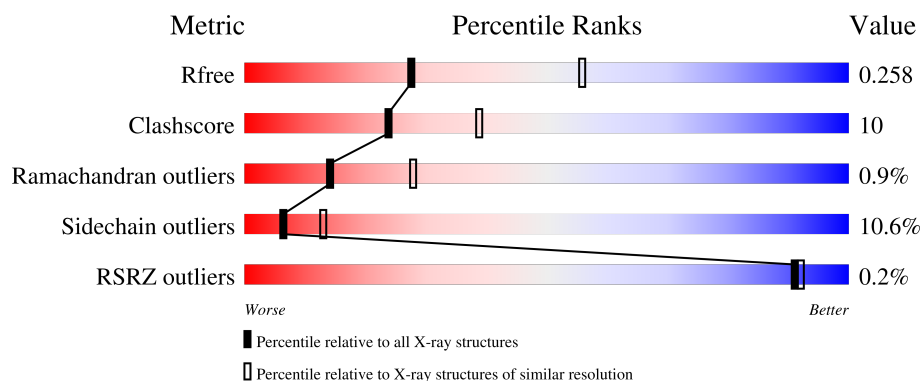
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	T	18	
2	P	14	
3	A	903	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8314 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 DNA chain called Template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	18	Total	C	N	O	P	0	0	0
			364	174	66	107	17			

- Molecule 2 is a DNA chain called Primer DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	14	Total	C	N	O	P	0	0	0
			286	137	55	81	13			

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	903	Total	C	N	O	S	0	0	0
			7350	4721	1220	1376	33			

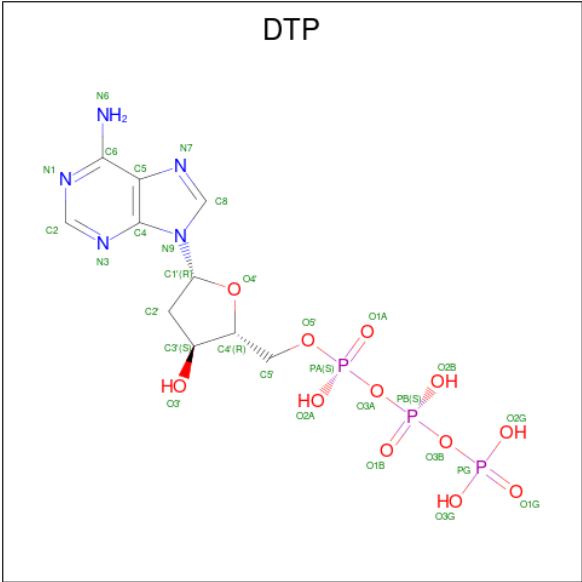
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	ALA	ASP	engineered mutation	UNP Q38087
A	327	ALA	ASP	engineered mutation	UNP Q38087

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

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

- Molecule 5 is 2'-DEOXYADENOSINE 5'-TRIPHOSPHATE (CCD ID: DTP) (formula: C₁₀H₁₆N₅O₁₂P₃)



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

- Molecule 6 is water.

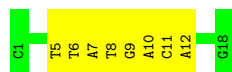
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	20	Total	O	0	0
			20	20		
6	P	29	Total	O	0	0
			29	29		
6	A	234	Total	O	0	0
			234	234		

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: Template DNA

Chain T:  56% 44%



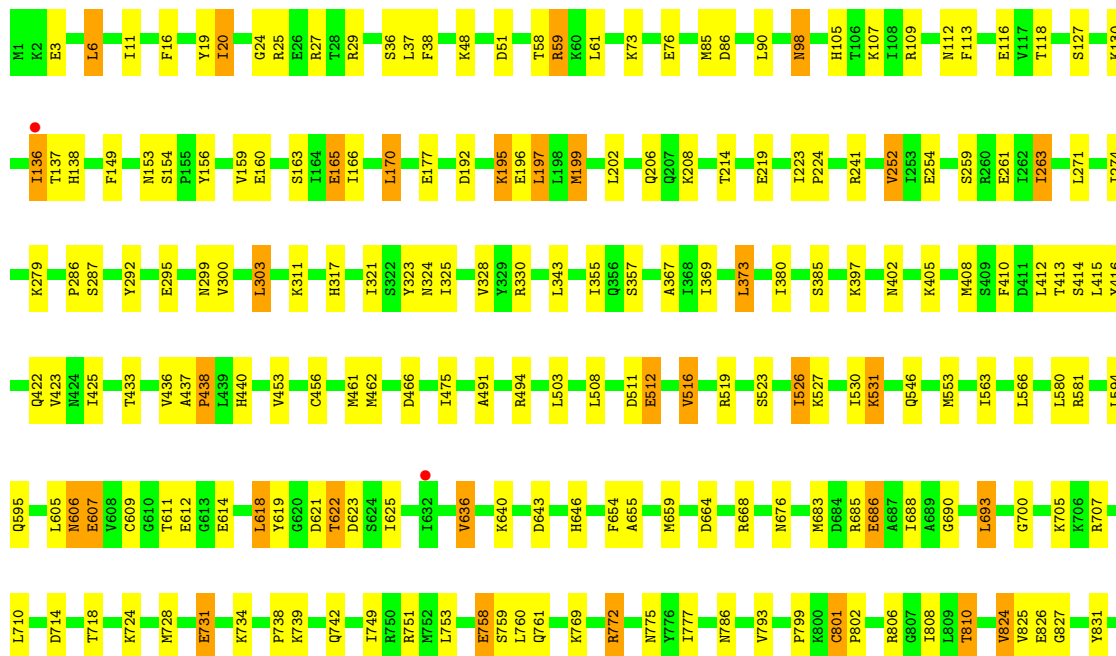
• Molecule 2: Primer DNA

Chain P:  57% 43%



• Molecule 3: DNA polymerase

Chain A:  74% 22% .



L835	R836	F841	A847	W848	T852	E853	I854	L857	I858	K859	D860	D861	V862	L863	L872	E873	K874	T875	F876	I877	K878	P879	L880	E881	T884	S885	L889	D890	Y891	S896	L897	F898	D899	M900	F901	D902	F903
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.31Å 117.75Å 129.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.75 30.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	92.5 (30.00-2.75) 87.3 (30.00-2.75)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.50 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.3.0011	Depositor
R, R_{free}	0.216 , 0.272 0.199 , 0.258	Depositor DCC
R_{free} test set	5998 reflections (9.65%)	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8314	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DDG, DTP, 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	T	0.42	0/407	1.15	0/626
2	P	0.40	0/297	1.09	0/457
3	A	0.60	0/7531	0.89	5/10182 (0.0%)
All	All	0.59	0/8235	0.91	5/11265 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	CYS	CA-C-N	6.68	126.64	120.03
3	A	801	CYS	C-N-CA	6.68	126.64	120.03
3	A	693	LEU	N-CA-C	5.28	118.00	110.24
3	A	113	PHE	N-CA-C	5.17	117.28	109.41
3	A	618	LEU	CA-CB-CG	5.03	133.89	116.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	364	0	204	6	0
2	P	286	0	159	6	0
3	A	7350	0	7212	146	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
5	A	30	0	12	2	0
6	A	234	0	0	16	0
6	P	29	0	0	5	0
6	T	20	0	0	0	0
All	All	8314	0	7587	157	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 10.

All (157) 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:A:195:LYS:HD2	3:A:195:LYS:H	1.10	1.12
3:A:373:LEU:HD23	3:A:380:ILE:HG22	1.51	0.89
1:T:10:DA:H2''	1:T:11:DC:H5''	1.56	0.86
3:A:606:ASN:HD21	3:A:614:GLU:HB2	1.38	0.86
3:A:195:LYS:HD2	3:A:195:LYS:N	1.93	0.79
1:T:7:DA:H5''	3:A:705:LYS:HD3	1.67	0.77
3:A:494:ARG:NH1	6:A:940:HOH:O	2.19	0.76
3:A:772:ARG:CG	3:A:772:ARG:HH11	2.01	0.74
3:A:440:HIS:HB3	6:A:939:HOH:O	1.90	0.71
3:A:136:ILE:HD11	3:A:138:HIS:HB2	1.71	0.71
3:A:286:PRO:HG2	3:A:292:TYR:OH	1.91	0.70
3:A:408:MET:CE	3:A:688:ILE:HG12	2.23	0.68
3:A:526:ILE:O	3:A:530:ILE:HG12	1.93	0.68
3:A:516:VAL:HG11	3:A:526:ILE:HD13	1.74	0.68
3:A:170:LEU:HA	3:A:177:GLU:HG3	1.75	0.67
3:A:109:ARG:NH1	3:A:208:LYS:HG2	2.09	0.67
3:A:896:SER:C	3:A:898:PHE:H	2.03	0.66
2:P:104:DG:H1'	6:P:131:HOH:O	1.96	0.65
3:A:223:ILE:HB	3:A:224:PRO:HD3	1.79	0.65
3:A:433:THR:O	3:A:462:MET:HE2	1.96	0.64
3:A:11:ILE:HD12	3:A:16:PHE:CD1	2.34	0.62
2:P:107:DG:H1'	6:P:139:HOH:O	1.99	0.62
3:A:654:PHE:CD2	3:A:659:MET:HE2	2.35	0.61
3:A:323:TYR:HE1	6:A:1119:HOH:O	1.83	0.61
3:A:475:ILE:HD12	3:A:566:LEU:HD23	1.83	0.61
3:A:739:LYS:NZ	6:A:1099:HOH:O	2.34	0.60
2:P:105:DC:H5'	6:P:131:HOH:O	2.02	0.60
3:A:686:GLU:HG2	6:A:962:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:416:TYR:CG	5:A:905:DTP:H2'1	2.38	0.58
1:T:5:DT:H1'	1:T:6:DT:H5'	1.85	0.58
3:A:37:LEU:C	3:A:38:PHE:CD1	2.82	0.58
3:A:397:LYS:HD3	3:A:619:TYR:HA	1.86	0.58
3:A:415:LEU:HD22	3:A:623:ASP:HB3	1.86	0.57
1:T:10:DA:C2'	1:T:11:DC:H5''	2.31	0.57
3:A:531:LYS:HD2	3:A:531:LYS:H	1.69	0.57
3:A:606:ASN:ND2	3:A:614:GLU:HB2	2.17	0.56
3:A:199:MET:HE2	3:A:241:ARG:NH2	2.20	0.56
3:A:878:LYS:HB2	3:A:879:PRO:HD3	1.88	0.56
3:A:149:PHE:HB3	3:A:197:LEU:HD13	1.87	0.55
3:A:685:ARG:HD2	3:A:685:ARG:C	2.31	0.55
3:A:25:ARG:CB	3:A:27:ARG:HH21	2.20	0.55
3:A:772:ARG:HH11	3:A:772:ARG:HG3	1.69	0.54
3:A:664:ASP:O	3:A:668:ARG:HG2	2.08	0.54
3:A:412:LEU:HD13	3:A:415:LEU:HD13	1.90	0.54
3:A:523:SER:O	3:A:526:ILE:HG23	2.08	0.54
3:A:303:LEU:HD12	3:A:303:LEU:H	1.72	0.54
3:A:195:LYS:H	3:A:195:LYS:CD	1.98	0.53
3:A:408:MET:HG2	3:A:410:PHE:CE1	2.42	0.53
3:A:793:VAL:HG12	3:A:793:VAL:O	2.08	0.53
3:A:199:MET:HE3	3:A:199:MET:HA	1.92	0.52
3:A:224:PRO:HA	3:A:263:ILE:HD13	1.91	0.52
3:A:772:ARG:HH11	3:A:772:ARG:HG2	1.73	0.52
3:A:772:ARG:CG	3:A:772:ARG:NH1	2.67	0.52
3:A:896:SER:C	3:A:898:PHE:N	2.66	0.52
3:A:516:VAL:HG11	3:A:526:ILE:CD1	2.39	0.51
3:A:884:THR:HG23	3:A:889:LEU:O	2.11	0.51
2:P:102:DC:H2'	2:P:103:DG:C8	2.46	0.51
3:A:321:ILE:O	3:A:325:ILE:HG13	2.10	0.51
3:A:437:ALA:O	3:A:438:PRO:C	2.53	0.51
3:A:38:PHE:CD1	3:A:38:PHE:N	2.79	0.51
3:A:605:LEU:O	3:A:609:CYS:HB2	2.11	0.50
3:A:854:ILE:HD13	3:A:859:LYS:HG3	1.92	0.50
3:A:90:LEU:HD13	3:A:367:ALA:HB2	1.94	0.50
3:A:202:LEU:HD22	3:A:241:ARG:HB2	1.94	0.49
3:A:605:LEU:O	3:A:609:CYS:CB	2.60	0.49
3:A:758:GLU:HB2	6:A:974:HOH:O	2.12	0.49
3:A:153:ASN:HB2	3:A:192:ASP:O	2.11	0.49
3:A:112:ASN:OD1	3:A:214:THR:HG23	2.12	0.49
2:P:102:DC:H2'	2:P:103:DG:N7	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:24:GLY:HA3	3:A:107:LYS:HE2	1.95	0.49
3:A:749:ILE:O	3:A:753:LEU:HG	2.12	0.49
3:A:872:LEU:O	3:A:877:ILE:HG13	2.14	0.48
2:P:102:DC:H4'	6:P:115:HOH:O	2.13	0.48
3:A:323:TYR:CE1	6:A:1119:HOH:O	2.56	0.48
3:A:408:MET:HE3	3:A:688:ILE:HG12	1.94	0.48
3:A:836:ARG:HB2	3:A:836:ARG:NH1	2.29	0.47
3:A:841:PHE:HZ	3:A:861:ASP:HB2	1.79	0.47
3:A:199:MET:HE2	3:A:241:ARG:HH21	1.79	0.47
3:A:654:PHE:HD2	3:A:659:MET:HE2	1.77	0.47
3:A:786:ASN:HD21	3:A:827:GLY:HA2	1.80	0.47
3:A:848:TRP:CG	3:A:854:ILE:HG23	2.50	0.47
3:A:808:ILE:HG23	3:A:824:VAL:HG11	1.95	0.47
3:A:405:LYS:O	3:A:690:GLY:HA2	2.14	0.47
3:A:786:ASN:ND2	3:A:827:GLY:HA2	2.30	0.47
3:A:408:MET:HE2	3:A:688:ILE:HG12	1.96	0.47
3:A:415:LEU:HD22	3:A:623:ASP:CB	2.44	0.47
3:A:707:ARG:HH22	3:A:731:GLU:CD	2.22	0.46
3:A:526:ILE:O	3:A:526:ILE:HG13	2.13	0.46
3:A:700:GLY:HA3	3:A:710:LEU:HD23	1.98	0.46
3:A:199:MET:CE	3:A:241:ARG:HH21	2.29	0.46
3:A:772:ARG:HG2	3:A:772:ARG:NH1	2.30	0.46
3:A:891:TYR:N	6:A:1118:HOH:O	2.47	0.46
3:A:423:VAL:HB	3:A:425:ILE:HG13	1.98	0.46
3:A:836:ARG:HH11	3:A:836:ARG:CB	2.29	0.46
3:A:854:ILE:CD1	3:A:859:LYS:HG3	2.45	0.46
3:A:693:LEU:HD13	6:A:943:HOH:O	2.15	0.46
3:A:416:TYR:CD2	5:A:905:DTP:H2'1	2.50	0.46
3:A:6:LEU:HD21	3:A:20:ILE:CD1	2.47	0.45
3:A:29:ARG:HD3	6:A:920:HOH:O	2.16	0.45
3:A:873:GLU:OE2	3:A:878:LYS:HG2	2.17	0.45
3:A:456:CYS:SG	3:A:462:MET:HG2	2.57	0.44
3:A:806:ARG:O	3:A:810:THR:HG23	2.16	0.44
3:A:105:HIS:HD2	6:A:908:HOH:O	1.99	0.44
3:A:369:ILE:O	3:A:373:LEU:HB2	2.16	0.44
3:A:422:GLN:O	3:A:676:ASN:HB3	2.17	0.44
3:A:461:MET:SD	3:A:581:ARG:HB3	2.57	0.44
3:A:621:ASP:O	3:A:623:ASP:N	2.49	0.44
3:A:622:THR:HA	6:A:1044:HOH:O	2.17	0.44
3:A:801:CYS:HA	3:A:802:PRO:HD3	1.71	0.44
3:A:165:GLU:HG3	3:A:166:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:874:LYS:HG3	3:A:875:THR:N	2.32	0.44
3:A:751:ARG:HG2	3:A:759:SER:OG	2.17	0.44
3:A:252:VAL:HG23	3:A:261:GLU:HG2	1.99	0.44
3:A:714:ASP:HA	3:A:718:THR:O	2.17	0.44
3:A:685:ARG:HH22	3:A:714:ASP:CG	2.25	0.43
3:A:899:ASP:C	3:A:901:PHE:H	2.25	0.43
3:A:738:PRO:O	3:A:742:GLN:HG3	2.18	0.43
3:A:36:SER:HB3	3:A:59:ARG:HG3	1.99	0.43
3:A:841:PHE:CZ	3:A:861:ASP:HB2	2.52	0.43
3:A:831:TYR:O	3:A:847:ALA:HA	2.19	0.43
3:A:775:ASN:ND2	3:A:777:ILE:HB	2.33	0.43
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.53	0.43
3:A:611:THR:HB	3:A:612:GLU:H	1.70	0.43
3:A:3:GLU:OE2	3:A:19:TYR:HE2	2.01	0.42
3:A:731:GLU:HG3	3:A:879:PRO:HB3	2.00	0.42
3:A:876:PHE:C	3:A:879:PRO:HD2	2.44	0.42
3:A:163:SER:HB3	3:A:166:ILE:HD12	2.01	0.42
3:A:491:ALA:HB3	3:A:519:ARG:O	2.19	0.42
3:A:693:LEU:HD23	3:A:693:LEU:HA	1.90	0.42
3:A:874:LYS:HG3	3:A:875:THR:HG23	2.00	0.42
3:A:899:ASP:C	3:A:901:PHE:N	2.77	0.42
3:A:137:THR:HB	3:A:328:VAL:HG21	2.00	0.42
3:A:373:LEU:HD12	3:A:373:LEU:HA	1.92	0.42
6:P:143:HOH:O	3:A:734:LYS:NZ	2.52	0.42
3:A:408:MET:HG2	3:A:410:PHE:HE1	1.82	0.42
3:A:154:SER:C	3:A:156:TYR:N	2.77	0.42
3:A:836:ARG:NH1	3:A:836:ARG:CB	2.83	0.42
3:A:858:ILE:O	3:A:862:VAL:HG12	2.20	0.42
3:A:51:ASP:C	3:A:51:ASP:OD1	2.63	0.42
3:A:761:GLN:HE21	3:A:761:GLN:HB2	1.68	0.41
1:T:8:DT:H2''	1:T:9:DG:O5'	2.19	0.41
3:A:625:ILE:HG12	3:A:683:MET:HE1	2.02	0.41
3:A:655:ALA:HA	3:A:659:MET:HE3	2.03	0.41
1:T:11:DC:H2''	1:T:12:DA:C8	2.55	0.41
3:A:271:LEU:HD11	3:A:355:ILE:HG22	2.02	0.41
3:A:105:HIS:CD2	6:A:908:HOH:O	2.74	0.41
3:A:511:ASP:HB2	3:A:512:GLU:H	1.63	0.41
3:A:799:PRO:C	3:A:801:CYS:H	2.29	0.41
3:A:311:LYS:HD2	6:A:1129:HOH:O	2.20	0.41
3:A:643:ASP:N	3:A:643:ASP:OD1	2.54	0.41
3:A:118:THR:HG23	6:A:1058:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:413:THR:O	3:A:414:SER:C	2.63	0.40
3:A:875:THR:O	3:A:879:PRO:HG2	2.22	0.40
3:A:25:ARG:HA	6:A:1040:HOH:O	2.22	0.40
3:A:775:ASN:HD21	3:A:777:ILE:HB	1.85	0.40
3:A:116:GLU:HG2	3:A:324:ASN:ND2	2.35	0.40
3:A:777:ILE:HD11	3:A:853:GLU:HG2	2.02	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	
3	A	901/903 (100%)	828 (92%)	65 (7%)	8 (1%)	14	28

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	466	ASP
3	A	254	GLU
3	A	98	ASN
3	A	897	LEU
3	A	607	GLU
3	A	622	THR
3	A	636	VAL
3	A	438	PRO

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
3	A	794/800 (99%)	710 (89%)	84 (11%)	6 13

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	6	LEU
3	A	20	ILE
3	A	48	LYS
3	A	58	THR
3	A	59	ARG
3	A	61	LEU
3	A	73	LYS
3	A	76	GLU
3	A	85	MET
3	A	86	ASP
3	A	98	ASN
3	A	127	SER
3	A	130	LYS
3	A	136	ILE
3	A	160	GLU
3	A	165	GLU
3	A	170	LEU
3	A	195	LYS
3	A	196	GLU
3	A	197	LEU
3	A	199	MET
3	A	206	GLN
3	A	219	GLU
3	A	252	VAL
3	A	259	SER
3	A	263	ILE
3	A	274	ILE
3	A	279	LYS
3	A	287	SER
3	A	295	GLU
3	A	299	ASN
3	A	300	VAL
3	A	303	LEU
3	A	330	ARG
3	A	343	LEU

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Mol	Chain	Res	Type
3	A	357	SER
3	A	373	LEU
3	A	385	SER
3	A	402	ASN
3	A	436	VAL
3	A	453	VAL
3	A	503	LEU
3	A	508	LEU
3	A	512	GLU
3	A	516	VAL
3	A	526	ILE
3	A	527	LYS
3	A	531	LYS
3	A	546	GLN
3	A	553	MET
3	A	563	ILE
3	A	580	LEU
3	A	594	LEU
3	A	595	GLN
3	A	606	ASN
3	A	607	GLU
3	A	618	LEU
3	A	636	VAL
3	A	640	LYS
3	A	646	HIS
3	A	686	GLU
3	A	724	LYS
3	A	728	MET
3	A	731	GLU
3	A	758	GLU
3	A	760	LEU
3	A	769	LYS
3	A	772	ARG
3	A	810	THR
3	A	824	VAL
3	A	825	VAL
3	A	826	GLU
3	A	835	LEU
3	A	852	THR
3	A	854	ILE
3	A	857	LEU
3	A	862	VAL

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Mol	Chain	Res	Type
3	A	863	LEU
3	A	880	LEU
3	A	881	GLU
3	A	884	THR
3	A	885	SER
3	A	889	LEU
3	A	897	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	98	ASN
3	A	105	HIS
3	A	153	ASN
3	A	206	GLN
3	A	228	ASN
3	A	299	ASN
3	A	354	GLN
3	A	402	ASN
3	A	485	HIS
3	A	539	ASN
3	A	564	ASN
3	A	582	ASN
3	A	595	GLN
3	A	646	HIS
3	A	676	ASN
3	A	742	GLN
3	A	761	GLN
3	A	786	ASN
3	A	812	ASN
3	A	818	ASN
3	A	823	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\# Z > 2$
2	DDG	P	114	1,2	20,23,24	0.46	0	27,33,36	0.96	2 (7%)

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
2	DDG	P	114	1,2	-	2/7/18/19	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	P	114	DDG	O4'-C1'-N9	2.91	113.03	107.86
2	P	114	DDG	C2'-C1'-N9	-2.57	107.53	112.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	P	114	DDG	O4'-C4'-C5'-O5'
2	P	114	DDG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 1 is 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$
5	DTP	A	905	4	31,32,32	1.36	6 (19%)	46,50,50	2.02	12 (26%)

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	DTP	A	905	4	-	3/22/34/34	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	905	DTP	C5-C4	4.20	1.46	1.39
5	A	905	DTP	C5-C6	2.85	1.48	1.41
5	A	905	DTP	C5-N7	-2.43	1.34	1.39
5	A	905	DTP	PB-O3B	2.07	1.61	1.59
5	A	905	DTP	C8-N7	2.03	1.35	1.31
5	A	905	DTP	C8-N9	-2.03	1.34	1.37

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	DTP	C5-C4-N3	-6.93	117.17	126.72
5	A	905	DTP	C4-C5-N7	-4.50	105.44	110.58
5	A	905	DTP	C2-N3-C4	4.42	122.62	111.83
5	A	905	DTP	N3-C2-N1	-4.23	122.17	128.58
5	A	905	DTP	N3-C4-N9	4.18	134.28	127.17
5	A	905	DTP	C5-C4-N9	2.51	108.55	105.81
5	A	905	DTP	C2-N1-C6	2.44	122.75	118.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	905	DTP	C5-N7-C8	2.36	107.16	103.45
5	A	905	DTP	C6-C5-N7	2.25	136.42	132.09
5	A	905	DTP	O4'-C1'-N9	2.23	111.96	107.96
5	A	905	DTP	C2'-C3'-C4'	-2.17	98.40	102.80
5	A	905	DTP	O2A-PA-O1A	2.09	122.16	112.44

There are no chirality outliers.

All (3) torsion outliers are listed below:

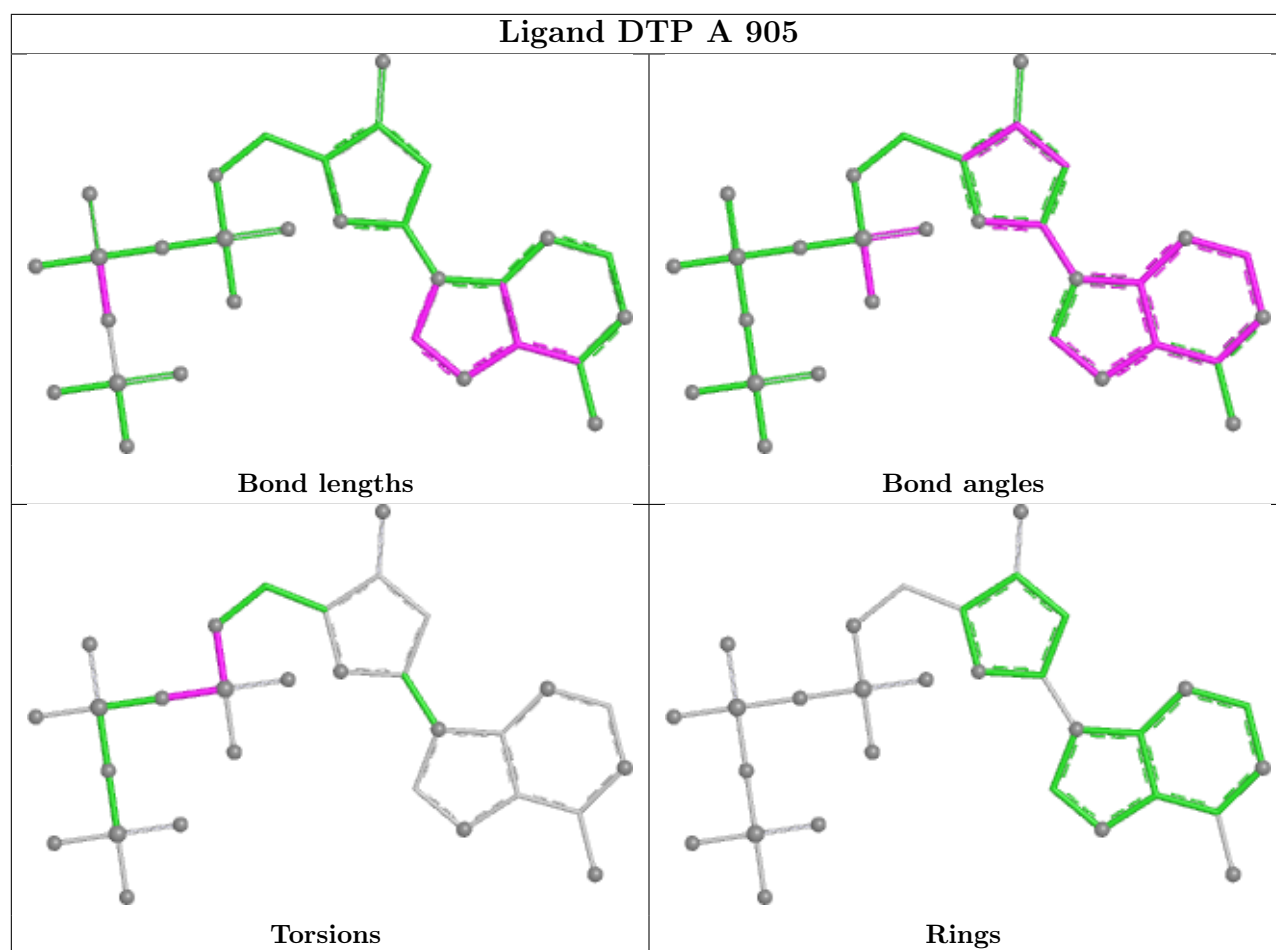
Mol	Chain	Res	Type	Atoms
5	A	905	DTP	C5'-O5'-PA-O2A
5	A	905	DTP	PB-O3A-PA-O5'
5	A	905	DTP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	905	DTP	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	T	18/18 (100%)	-0.54	0 100 100	33, 49, 82, 103	0
2	P	13/14 (92%)	-0.41	0 100 100	39, 45, 95, 95	0
3	A	903/903 (100%)	-0.05	2 (0%) 91 92	39, 60, 80, 103	0
All	All	934/935 (99%)	-0.07	2 (0%) 91 92	33, 59, 81, 103	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	136	ILE	2.3
3	A	632	ILE	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	DDG	P	114	21/22	0.96	0.07	43,45,47,48	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

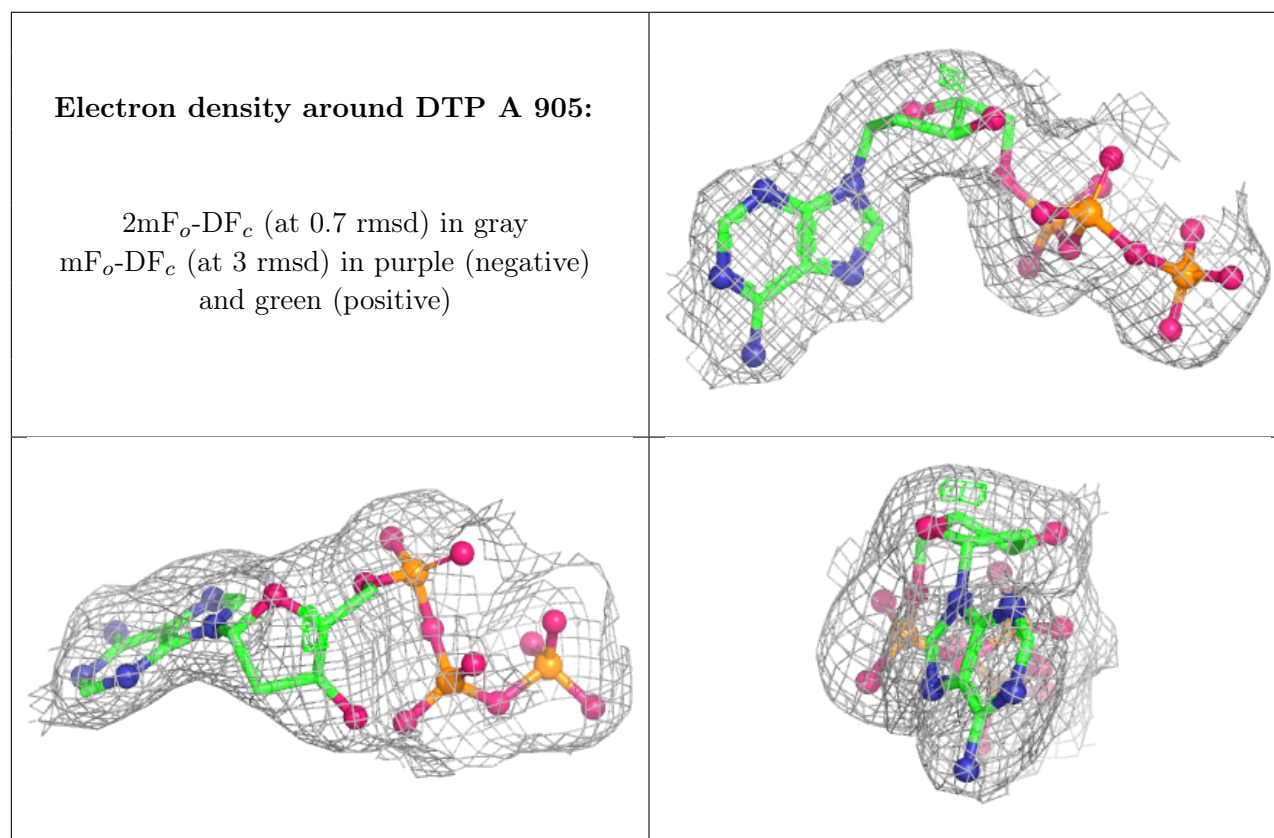
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
5	DTP	A	905	30/30	0.97	0.05	27,34,40,40	0
4	MG	A	904	1/1	1.00	0.02	44,44,44,44	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.