



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 04:09 AM EDT

PDB ID : 3CQ8  
Title : Ternary complex of the L415F mutant RB69 exo(-)polymerase  
Authors : Zhong, X.; Pedersen, L.C.; Kunkel, T.A.  
Deposited on : 2008-04-02  
Resolution : 2.50 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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

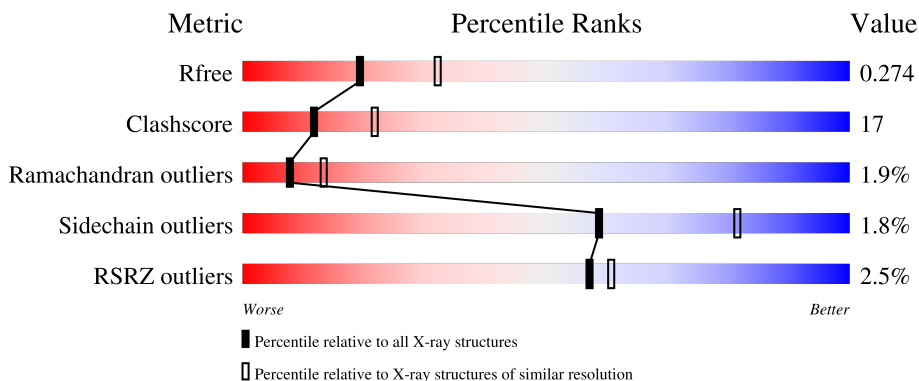
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	

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
7	GOL	A	1100	-	X	-	-
7	GOL	A	1101	-	X	-	-
7	GOL	A	1102	-	X	-	-

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8484 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 DNA (5'-D(\*DAP\*DCP\*DAP\*DGP\*DGP\*DTP\*DAP\*DAP\*DGP\*DCP\*DAP\*DGP\*DTP\*DCP\*DCP\*DGP\*DCP\*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	T	18	369	175	74	103	17	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(\*DGP\*DCP\*DGP\*DGP\*DAP\*DCP\*DTP\*DGP\*DCP\*DTP\*DTP\*DAP\*DCP\*DC)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	P	14	281	135	51	82	13	0	0	0

- Molecule 3 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	902	7345	4720	1219	1373	33	0	0	0

There are 3 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
A	415	PHE	LEU	engineered mutation	UNP Q38087

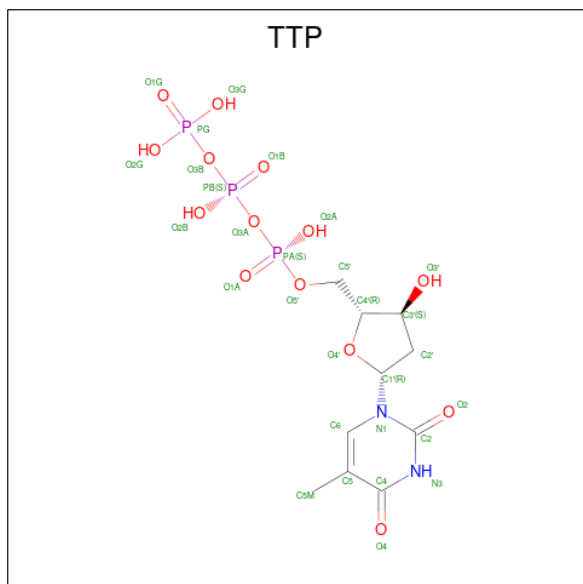
- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	Ca	0	0
			6	6		

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

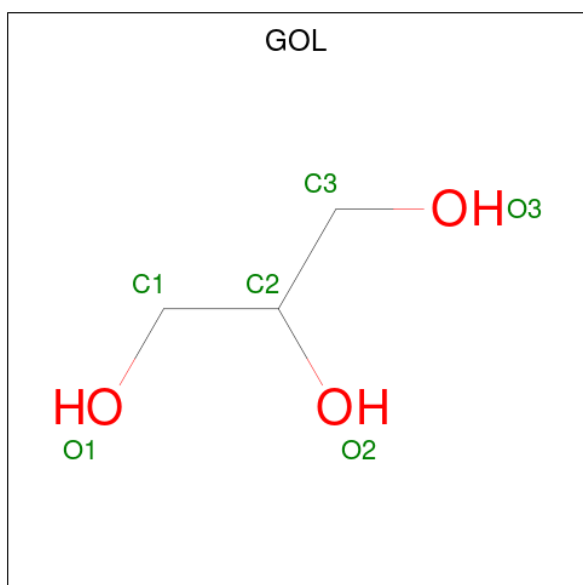
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	Na	0	0
			3	3		

- Molecule 6 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula:  $C_{10}H_{17}N_2O_{14}P_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
6	A	1	29	10	2	14	3	0	0

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0
7	A	1	Total C O 6 3 3	0	0

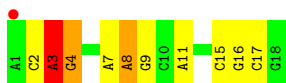
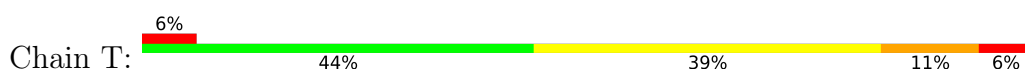
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	T	28	Total O 28 28	0	0
8	P	16	Total O 16 16	0	0
8	A	389	Total O 389 389	0	0

### 3 Residue-property plots

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.

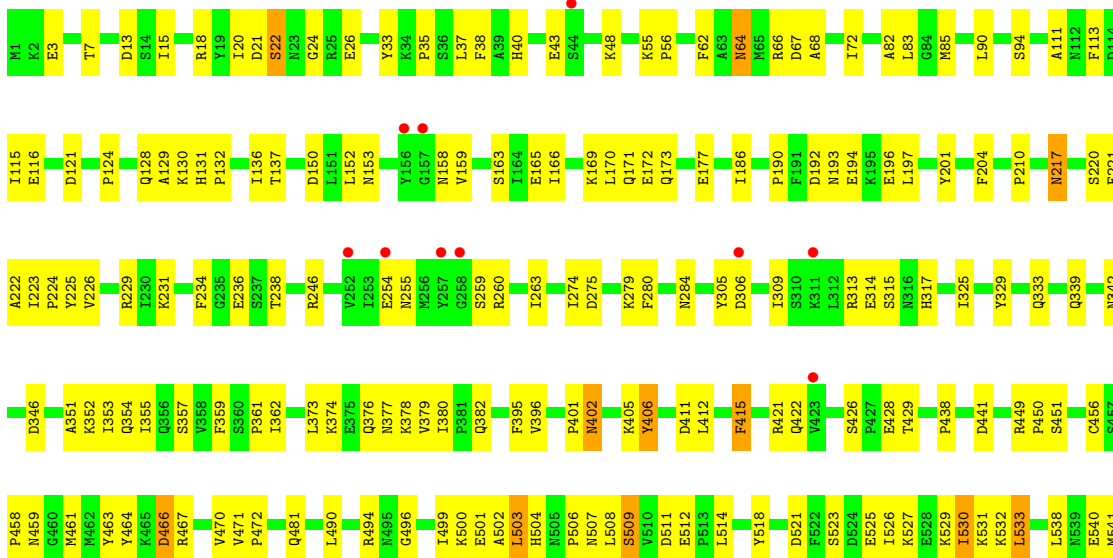
- Molecule 1: DNA (5'-D(\*DAP\*DCP\*DAP\*DGP\*DGP\*DTP\*DAP\*DAP\*DGP\*DCP\*DAP\*DG\*P\*DTP\*DCP\*DCP\*DGP\*DCP\*DG)-3')

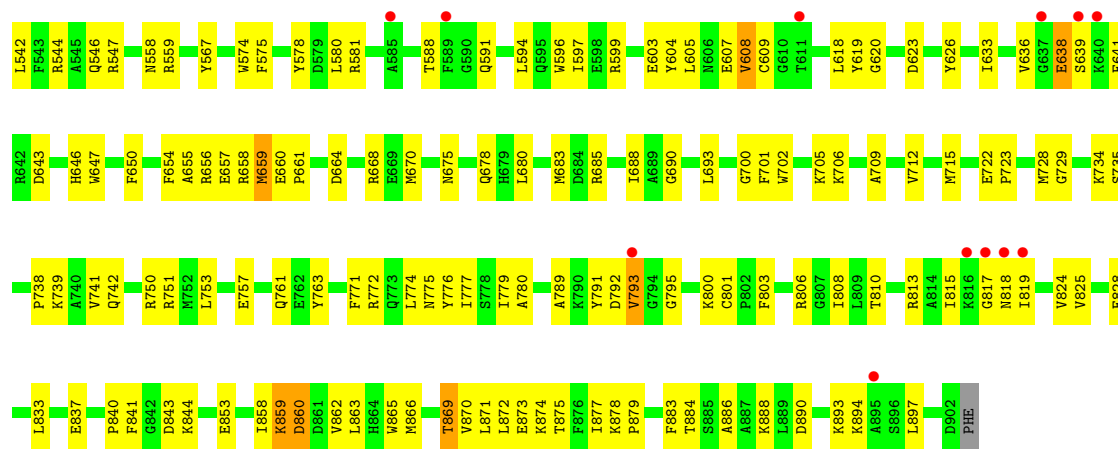


- Molecule 2: DNA (5'-D(\*DGP\*DCP\*DGP\*DGP\*DAP\*DCP\*DTP\*DGP\*DCP\*DTP\*DTP\*DA\*P\*DCP\*DC)-3')



- Molecule 3: DNA polymerase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.84Å 117.01Å 127.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.70 – 2.50 25.70 – 2.49	Depositor EDS
% Data completeness (in resolution range)	79.8 (25.70-2.50) 79.5 (25.70-2.49)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.50Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.212 , 0.281 0.204 , 0.274	Depositor DCC
$R_{free}$ test set	2110 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.1	Xtrriage
Anisotropy	0.278	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8484	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: GOL, CA, TTP, NA

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	0.44	0/415	0.78	1/639 (0.2%)
2	P	0.44	0/314	0.69	0/482
3	A	0.38	0/7526	0.60	0/10174
All	All	0.38	0/8255	0.61	1/11295 (0.0%)

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	T	0	3
2	P	0	1
All	All	0	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	3	DA	N9-C1'-C2'	-5.14	102.83	112.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	P	112	DT	Sidechain
1	T	3	DA	Sidechain
1	T	4	DG	Sidechain
1	T	8	DA	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	T	369	0	202	14	0
2	P	281	0	157	9	0
3	A	7345	0	7213	259	0
4	A	6	0	0	0	0
5	A	3	0	0	0	0
6	A	29	0	13	0	0
7	A	18	0	18	2	0
8	A	389	0	0	17	0
8	P	16	0	0	0	0
8	T	28	0	0	0	0
All	All	8484	0	7603	272	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 17.

All (272) 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:712:VAL:HG11	3:A:715:MET:HE2	1.46	0.95
3:A:373:LEU:HD21	3:A:470:VAL:HG21	1.53	0.91
3:A:428:GLU:OE2	3:A:470:VAL:HG23	1.71	0.89
2:P:114:DC:H2''	2:P:115:DC:H5''	1.54	0.89
3:A:481:GLN:HB3	3:A:559:ARG:HD3	1.59	0.83
3:A:700:GLY:H	3:A:753:LEU:HD22	1.46	0.79
3:A:825:VAL:HB	3:A:828:GLU:CG	2.15	0.77
3:A:373:LEU:HD12	3:A:380:ILE:HG22	1.66	0.76
3:A:862:VAL:O	3:A:866:MET:HG3	1.86	0.76
3:A:641:PHE:HA	3:A:646:HIS:ND1	2.01	0.76
3:A:772:ARG:NH2	3:A:869:THR:HG23	2.01	0.76
3:A:712:VAL:HG11	3:A:715:MET:CE	2.16	0.75
3:A:507:ASN:HB2	3:A:532:LYS:O	1.88	0.74
3:A:514:LEU:CD1	3:A:533:LEU:HD11	2.18	0.73
3:A:757:GLU:HG2	3:A:761:GLN:HE21	1.53	0.72
3:A:604:TYR:O	3:A:608:VAL:HG22	1.90	0.71
3:A:449:ARG:HH21	3:A:675:ASN:HB2	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:789:ALA:HA	3:A:792:ASP:HB2	1.72	0.70
3:A:825:VAL:HB	3:A:828:GLU:HG3	1.74	0.69
1:T:16:DG:H2''	1:T:17:DC:C5'	2.24	0.68
3:A:401:PRO:O	3:A:402:ASN:HB2	1.91	0.68
3:A:878:LYS:HB3	3:A:879:PRO:HD3	1.75	0.68
3:A:817:GLY:O	3:A:819:ILE:HG13	1.94	0.68
1:T:2:DC:H5'	3:A:574:TRP:CD1	2.30	0.67
2:P:113:DA:C5'	3:A:734:LYS:HG2	2.24	0.67
3:A:803:PHE:HE1	3:A:844:LYS:HE3	1.61	0.67
3:A:128:GLN:HG2	3:A:130:LYS:HE3	1.77	0.66
3:A:395:PHE:HB2	3:A:591:GLN:HG2	1.76	0.66
3:A:757:GLU:HG2	3:A:761:GLN:NE2	2.11	0.65
3:A:825:VAL:HB	3:A:828:GLU:HG2	1.78	0.65
1:T:11:DA:OP1	3:A:874:LYS:HE3	1.98	0.64
3:A:738:PRO:HD2	3:A:875:THR:HG21	1.79	0.64
3:A:775:ASN:ND2	8:A:1327:HOH:O	2.10	0.64
2:P:114:DC:C2'	2:P:115:DC:H5''	2.26	0.63
3:A:170:LEU:HA	3:A:177:GLU:HG3	1.79	0.63
3:A:373:LEU:HD21	3:A:470:VAL:CG2	2.27	0.63
3:A:405:LYS:O	3:A:690:GLY:HA2	1.99	0.63
2:P:114:DC:H2''	2:P:115:DC:C5'	2.28	0.62
3:A:523:SER:O	3:A:527:LYS:HG3	1.99	0.62
3:A:396:VAL:O	3:A:705:LYS:HE2	1.99	0.62
3:A:471:VAL:HB	3:A:472:PRO:HD3	1.81	0.61
3:A:159:VAL:HG21	3:A:317:HIS:CG	2.35	0.61
3:A:815:ILE:CG2	3:A:858:ILE:HD11	2.30	0.61
3:A:860:ASP:HA	3:A:863:LEU:HD12	1.82	0.61
3:A:859:LYS:HG2	3:A:863:LEU:HD11	1.83	0.60
3:A:159:VAL:HG21	3:A:317:HIS:CD2	2.36	0.60
3:A:415:PHE:CD2	3:A:623:ASP:HB3	2.35	0.60
3:A:514:LEU:HD13	3:A:533:LEU:HD11	1.81	0.60
3:A:607:GLU:C	3:A:609:CYS:H	2.05	0.60
3:A:163:SER:OG	3:A:166:ILE:HG12	2.02	0.60
3:A:806:ARG:O	3:A:810:THR:HG23	2.02	0.60
3:A:741:VAL:HG11	3:A:875:THR:HG22	1.84	0.60
1:T:3:DA:OP2	3:A:361:PRO:HD2	2.02	0.59
3:A:171:GLN:N	3:A:177:GLU:HG3	2.17	0.59
3:A:870:VAL:CG1	3:A:874:LYS:HD3	2.32	0.59
3:A:197:LEU:HD23	3:A:197:LEU:C	2.23	0.59
2:P:113:DA:H5'	3:A:734:LYS:HG2	1.85	0.59
3:A:153:ASN:HB2	3:A:192:ASP:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:171:GLN:H	3:A:177:GLU:HG3	1.68	0.59
3:A:793:VAL:HG12	3:A:793:VAL:O	2.03	0.59
3:A:738:PRO:HG3	3:A:780:ALA:O	2.03	0.58
3:A:860:ASP:HB2	8:A:1255:HOH:O	2.02	0.58
3:A:217:ASN:HD22	3:A:220:SER:HB2	1.69	0.58
3:A:897:LEU:HB3	8:A:1267:HOH:O	2.05	0.57
3:A:496:GLY:O	3:A:500:LYS:HG3	2.03	0.57
3:A:643:ASP:C	3:A:693:LEU:HD12	2.23	0.57
3:A:48:LYS:HE3	3:A:377:ASN:OD1	2.03	0.57
3:A:115:ILE:HG22	3:A:136:ILE:HG12	1.86	0.57
1:T:16:DG:H2''	1:T:17:DC:H5'	1.86	0.57
3:A:169:LYS:HD3	3:A:173:GLN:HG2	1.86	0.57
3:A:466:ASP:OD1	3:A:467:ARG:HG3	2.04	0.57
3:A:751:ARG:NE	3:A:763:TYR:HB2	2.20	0.56
3:A:362:ILE:HG23	3:A:575:PHE:HD1	1.71	0.56
3:A:458:PRO:HG2	3:A:588:THR:HG22	1.86	0.56
3:A:599:ARG:O	3:A:603:GLU:HG3	2.04	0.56
3:A:64:ASN:HD21	3:A:67:ASP:CG	2.09	0.56
3:A:422:GLN:HG3	3:A:678:GLN:O	2.06	0.56
1:T:16:DG:H2''	1:T:17:DC:H5''	1.88	0.56
3:A:246:ARG:HD2	8:A:1192:HOH:O	2.06	0.56
3:A:502:ALA:C	3:A:504:HIS:H	2.09	0.55
3:A:428:GLU:OE1	3:A:428:GLU:N	2.32	0.55
3:A:540:GLU:O	3:A:544:ARG:HG3	2.06	0.55
3:A:870:VAL:HG13	3:A:874:LYS:HD3	1.89	0.55
3:A:329:TYR:CE1	7:A:1101:GOL:H32	2.42	0.54
3:A:193:ASN:HD21	3:A:196:GLU:HG3	1.73	0.54
3:A:702:TRP:O	3:A:886:ALA:HB1	2.07	0.54
3:A:263:ILE:HD12	3:A:263:ILE:N	2.23	0.54
3:A:738:PRO:HD2	3:A:875:THR:CG2	2.37	0.54
3:A:405:LYS:HB3	3:A:406:TYR:HD2	1.72	0.54
3:A:795:GLY:O	3:A:813:ARG:NH1	2.40	0.53
3:A:512:GLU:OE1	3:A:512:GLU:HA	2.08	0.53
3:A:514:LEU:CD2	3:A:526:ILE:HG23	2.38	0.53
3:A:817:GLY:O	3:A:819:ILE:N	2.42	0.53
3:A:451:SER:HB3	3:A:456:CYS:SG	2.49	0.53
3:A:668:ARG:NH1	3:A:668:ARG:HG2	2.24	0.53
3:A:605:LEU:O	3:A:609:CYS:HB3	2.09	0.53
3:A:507:ASN:OD1	3:A:532:LYS:HA	2.08	0.53
3:A:15:ILE:HG22	3:A:15:ILE:O	2.09	0.52
3:A:342:ASN:HB2	7:A:1100:GOL:H31	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:858:ILE:HG22	3:A:862:VAL:CG1	2.40	0.52
3:A:530:ILE:HG23	3:A:538:LEU:HD21	1.91	0.52
3:A:841:PHE:HE1	3:A:858:ILE:HG23	1.74	0.52
3:A:658:ARG:O	3:A:661:PRO:HD2	2.10	0.52
3:A:668:ARG:HG2	3:A:668:ARG:HH11	1.74	0.52
3:A:411:ASP:OD2	3:A:412:LEU:N	2.42	0.52
3:A:547:ARG:NH2	8:A:1261:HOH:O	2.42	0.51
3:A:217:ASN:ND2	3:A:220:SER:HB2	2.25	0.51
3:A:657:GLU:O	3:A:661:PRO:HG2	2.10	0.51
3:A:499:ILE:O	3:A:502:ALA:HB3	2.11	0.51
3:A:514:LEU:HD23	3:A:526:ILE:HG23	1.92	0.51
3:A:150:ASP:OD2	3:A:317:HIS:CE1	2.63	0.51
3:A:502:ALA:O	3:A:504:HIS:N	2.37	0.51
3:A:33:TYR:O	3:A:35:PRO:HD3	2.11	0.51
3:A:223:ILE:N	3:A:224:PRO:HD2	2.26	0.51
3:A:775:ASN:HB2	8:A:1125:HOH:O	2.09	0.51
3:A:840:PRO:HD2	3:A:865:TRP:CD1	2.45	0.51
3:A:508:LEU:O	3:A:509:SER:HB3	2.11	0.50
3:A:506:PRO:HG2	8:A:1124:HOH:O	2.10	0.50
3:A:678:GLN:HG2	3:A:680:LEU:HG	1.94	0.50
3:A:305:TYR:OH	3:A:309:ILE:HB	2.11	0.50
3:A:193:ASN:HD21	3:A:196:GLU:CD	2.15	0.50
3:A:234:PHE:CB	3:A:238:THR:HG21	2.42	0.50
3:A:481:GLN:HB3	3:A:559:ARG:CD	2.36	0.50
3:A:406:TYR:CD1	3:A:633:ILE:HG13	2.47	0.49
3:A:701:PHE:CD1	3:A:753:LEU:HD21	2.47	0.49
3:A:527:LYS:O	3:A:531:LYS:HG3	2.12	0.49
3:A:43:GLU:HG2	3:A:56:PRO:HG3	1.93	0.49
3:A:83:LEU:HD12	3:A:83:LEU:H	1.77	0.49
3:A:525:GLU:O	3:A:529:LYS:HG3	2.12	0.49
3:A:193:ASN:ND2	3:A:196:GLU:HG3	2.28	0.49
3:A:279:LYS:HE3	3:A:359:PHE:O	2.12	0.49
3:A:619:TYR:CG	3:A:620:GLY:N	2.81	0.49
3:A:201:TYR:O	3:A:204:PHE:HB3	2.11	0.49
3:A:841:PHE:CE1	3:A:858:ILE:HG23	2.48	0.49
3:A:62:PHE:CE2	3:A:68:ALA:HA	2.48	0.48
3:A:618:LEU:HD12	3:A:619:TYR:N	2.28	0.48
3:A:761:GLN:OE1	3:A:893:LYS:HB2	2.13	0.48
3:A:401:PRO:O	3:A:402:ASN:CB	2.61	0.48
3:A:354:GLN:O	3:A:357:SER:HB2	2.14	0.48
3:A:438:PRO:HD2	3:A:441:ASP:OD2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:738:PRO:HB3	3:A:779:ILE:HA	1.94	0.48
3:A:3:GLU:HG2	3:A:22:SER:N	2.28	0.48
3:A:792:ASP:HB3	8:A:1281:HOH:O	2.13	0.48
3:A:449:ARG:NH2	3:A:675:ASN:HB2	2.26	0.48
3:A:618:LEU:HD12	3:A:619:TYR:CB	2.43	0.48
1:T:16:DG:C2'	1:T:17:DC:H5''	2.43	0.48
3:A:700:GLY:HA2	3:A:709:ALA:O	2.13	0.48
3:A:654:PHE:O	3:A:658:ARG:HB2	2.14	0.47
3:A:859:LYS:HG2	3:A:863:LEU:CD1	2.43	0.47
3:A:132:PRO:HB3	3:A:194:GLU:OE2	2.14	0.47
3:A:159:VAL:HG11	3:A:317:HIS:HB2	1.95	0.47
3:A:503:LEU:HD21	3:A:538:LEU:HB3	1.97	0.47
3:A:62:PHE:CD2	3:A:68:ALA:HA	2.49	0.47
3:A:841:PHE:CZ	3:A:862:VAL:HG12	2.49	0.47
3:A:664:ASP:HB3	8:A:1259:HOH:O	2.14	0.47
3:A:647:TRP:HA	3:A:650:PHE:HB3	1.96	0.47
2:P:114:DC:H3'	3:A:728:MET:HE2	1.95	0.47
3:A:791:TYR:CD2	3:A:801:CYS:HA	2.50	0.47
3:A:68:ALA:O	3:A:72:ILE:HG13	2.15	0.46
3:A:83:LEU:HB3	3:A:379:VAL:HG12	1.96	0.46
3:A:547:ARG:HD3	3:A:547:ARG:HA	1.80	0.46
3:A:858:ILE:HG22	3:A:862:VAL:HG13	1.96	0.46
3:A:609:CYS:HB2	8:A:1266:HOH:O	2.16	0.46
3:A:124:PRO:HB3	3:A:131:HIS:HD2	1.80	0.46
3:A:260:ARG:HG3	3:A:260:ARG:HH11	1.80	0.46
3:A:40:HIS:CD2	3:A:55:LYS:HE3	2.51	0.46
3:A:21:ASP:O	3:A:24:GLY:N	2.48	0.46
3:A:596:TRP:CE2	3:A:670:MET:HB2	2.50	0.46
3:A:837:GLU:O	3:A:837:GLU:HG3	2.15	0.46
3:A:13:ASP:OD1	3:A:66:ARG:HG3	2.16	0.46
3:A:82:ALA:O	3:A:382:GLN:HB2	2.16	0.46
3:A:607:GLU:O	3:A:609:CYS:N	2.48	0.46
3:A:660:GLU:HB2	3:A:661:PRO:HD3	1.97	0.46
3:A:313:ARG:HD3	8:A:1172:HOH:O	2.16	0.46
3:A:137:THR:HG21	3:A:325:ILE:HA	1.98	0.45
3:A:172:GLU:H	3:A:172:GLU:CD	2.18	0.45
3:A:873:GLU:OE2	3:A:877:ILE:HD12	2.16	0.45
3:A:884:THR:O	3:A:888:LYS:N	2.49	0.45
3:A:607:GLU:HG2	3:A:608:VAL:N	2.30	0.45
1:T:3:DA:H2''	1:T:4:DG:O5'	2.17	0.45
3:A:20:ILE:HD13	3:A:26:GLU:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:654:PHE:CD2	3:A:658:ARG:HG3	2.52	0.45
3:A:193:ASN:HD21	3:A:196:GLU:CG	2.28	0.45
3:A:193:ASN:OD1	3:A:196:GLU:HG3	2.17	0.45
3:A:186:ILE:HD13	3:A:325:ILE:HD13	1.97	0.45
3:A:638:GLU:HA	3:A:641:PHE:HD1	1.80	0.45
3:A:578:TYR:CZ	3:A:580:LEU:HD13	2.52	0.45
3:A:314:GLU:HG3	3:A:315:SER:H	1.81	0.45
3:A:406:TYR:N	3:A:406:TYR:CD2	2.83	0.45
3:A:429:THR:O	3:A:463:TYR:HA	2.17	0.45
3:A:833:LEU:HD22	3:A:871:LEU:HD11	1.99	0.45
3:A:152:LEU:HD11	3:A:190:PRO:HB2	1.99	0.45
3:A:284:ASN:O	3:A:735:SER:HB3	2.16	0.45
3:A:501:GLU:HA	3:A:504:HIS:CE1	2.52	0.45
3:A:815:ILE:HG22	3:A:858:ILE:HD11	1.97	0.45
3:A:329:TYR:O	3:A:333:GLN:HG3	2.17	0.44
2:P:109:DG:H5'	3:A:800:LYS:HE3	1.98	0.44
1:T:11:DA:H4'	3:A:803:PHE:HB2	1.99	0.44
3:A:165:GLU:O	3:A:169:LYS:HG3	2.17	0.44
3:A:739:LYS:HE2	3:A:739:LYS:HA	2.00	0.44
3:A:351:ALA:O	3:A:352:LYS:HB2	2.17	0.44
3:A:771:PHE:CG	3:A:872:LEU:HD13	2.52	0.44
3:A:90:LEU:HD21	3:A:353:ILE:HG22	2.00	0.44
3:A:222:ALA:O	3:A:226:VAL:HG23	2.18	0.44
3:A:37:LEU:C	3:A:38:PHE:CD1	2.91	0.44
3:A:872:LEU:O	3:A:877:ILE:HG13	2.17	0.44
3:A:153:ASN:HA	3:A:158:ASN:ND2	2.33	0.44
3:A:234:PHE:HB2	3:A:238:THR:HG21	2.00	0.43
1:T:15:DC:H2''	1:T:16:DG:C8	2.52	0.43
1:T:7:DA:H5''	3:A:705:LYS:HD3	2.00	0.43
3:A:655:ALA:HA	3:A:659:MET:CG	2.49	0.43
3:A:64:ASN:N	3:A:64:ASN:HD22	2.16	0.43
3:A:607:GLU:C	3:A:609:CYS:N	2.72	0.43
1:T:8:DA:H2''	1:T:9:DG:C8	2.53	0.43
3:A:152:LEU:O	3:A:158:ASN:HA	2.19	0.43
3:A:221:PHE:O	3:A:224:PRO:HG2	2.18	0.43
2:P:102:DG:H2''	2:P:103:DC:O5'	2.18	0.43
3:A:111:ALA:HB3	3:A:210:PRO:HB3	2.01	0.43
3:A:490:LEU:O	3:A:494:ARG:HG3	2.19	0.43
3:A:64:ASN:HD22	3:A:64:ASN:C	2.19	0.43
3:A:280:PHE:HB3	3:A:558:ASN:HD21	1.84	0.43
3:A:94:SER:OG	3:A:374:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:274:ILE:HG23	3:A:275:ASP:N	2.34	0.42
3:A:883:PHE:N	3:A:883:PHE:CD1	2.86	0.42
3:A:355:ILE:HG12	8:A:1354:HOH:O	2.20	0.42
3:A:461:MET:HE2	3:A:581:ARG:HB3	2.01	0.42
3:A:464:TYR:CD1	3:A:467:ARG:HD2	2.54	0.42
3:A:618:LEU:HD12	3:A:619:TYR:HB2	2.00	0.42
3:A:750:ARG:HH11	3:A:750:ARG:HG2	1.84	0.42
3:A:808:ILE:HG23	3:A:824:VAL:HG21	2.01	0.42
3:A:313:ARG:NH1	8:A:1419:HOH:O	2.52	0.42
3:A:777:ILE:CD1	3:A:853:GLU:HG2	2.49	0.42
3:A:83:LEU:HD12	3:A:83:LEU:N	2.34	0.42
3:A:426:SER:HB2	3:A:472:PRO:HD3	2.02	0.42
3:A:706:LYS:O	3:A:729:GLY:HA3	2.20	0.42
3:A:722:GLU:CD	3:A:723:PRO:HD2	2.40	0.42
3:A:772:ARG:HH21	3:A:869:THR:HG23	1.78	0.42
3:A:803:PHE:O	3:A:806:ARG:HB3	2.20	0.42
3:A:803:PHE:CE1	3:A:844:LYS:HE3	2.47	0.42
1:T:16:DG:H1'	1:T:17:DC:H5''	2.01	0.41
3:A:412:LEU:CD2	3:A:683:MET:HB2	2.49	0.41
3:A:231:LYS:HD2	3:A:236:GLU:HG3	2.02	0.41
3:A:421:ARG:NH2	8:A:1302:HOH:O	2.43	0.41
3:A:656:ARG:NE	8:A:1455:HOH:O	2.50	0.41
3:A:890:ASP:OD1	3:A:894:LYS:HE2	2.20	0.41
3:A:170:LEU:HA	3:A:177:GLU:CG	2.48	0.41
3:A:339:GLN:HG2	8:A:1308:HOH:O	2.19	0.41
3:A:734:LYS:O	3:A:742:GLN:NE2	2.53	0.41
3:A:194:GLU:OE1	3:A:229:ARG:NE	2.50	0.41
3:A:594:LEU:O	3:A:597:ILE:HG22	2.20	0.41
3:A:90:LEU:CD2	3:A:353:ILE:HG22	2.50	0.41
3:A:254:GLU:HA	3:A:259:SER:HA	2.02	0.41
3:A:618:LEU:HG	3:A:626:TYR:O	2.20	0.41
2:P:113:DA:H5''	3:A:734:LYS:HA	2.03	0.41
1:T:3:DA:H2''	1:T:4:DG:C5'	2.50	0.41
3:A:163:SER:HA	8:A:1285:HOH:O	2.21	0.41
3:A:494:ARG:HH21	3:A:521:ASP:CG	2.24	0.41
3:A:518:TYR:OH	3:A:541:MET:HG2	2.20	0.41
3:A:636:VAL:HG12	3:A:636:VAL:O	2.21	0.41
3:A:685:ARG:NH1	3:A:688:ILE:HD11	2.36	0.41
3:A:741:VAL:HG21	3:A:875:THR:CG2	2.51	0.41
3:A:776:TYR:CZ	3:A:777:ILE:HG13	2.56	0.41
3:A:542:LEU:O	3:A:546:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:376:GLN:HB3	3:A:378:LYS:HE3	2.01	0.40
3:A:412:LEU:HD12	3:A:623:ASP:HB2	2.04	0.40
3:A:777:ILE:HD11	3:A:853:GLU:HG2	2.03	0.40
3:A:129:ALA:HA	3:A:225:TYR:CZ	2.57	0.40
3:A:654:PHE:CE2	3:A:658:ARG:HG3	2.56	0.40
3:A:771:PHE:CD1	3:A:774:LEU:HD12	2.56	0.40
3:A:7:THR:OG1	3:A:18:ARG:HD3	2.22	0.40
3:A:85:MET:HA	3:A:380:ILE:HD11	2.02	0.40
3:A:618:LEU:HD12	3:A:618:LEU:C	2.41	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	900/903 (100%)	793 (88%)	90 (10%)	17 (2%)	<b>8</b>   <b>13</b>

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	121	ASP
3	A	608	VAL
3	A	818	ASN
3	A	306	ASP
3	A	402	ASN
3	A	503	LEU
3	A	530	ILE
3	A	639	SER
3	A	859	LYS
3	A	659	MET
3	A	22	SER
3	A	415	PHE

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Mol	Chain	Res	Type
3	A	255	ASN
3	A	509	SER
3	A	533	LEU
3	A	793	VAL
3	A	450	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	793/800 (99%)	779 (98%)	14 (2%)	59 81

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	64	ASN
3	A	113	PHE
3	A	116	GLU
3	A	217	ASN
3	A	346	ASP
3	A	406	TYR
3	A	459	ASN
3	A	466	ASP
3	A	511	ASP
3	A	567	TYR
3	A	638	GLU
3	A	843	ASP
3	A	860	ASP
3	A	869	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	64	ASN
3	A	70	GLN

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Mol	Chain	Res	Type
3	A	153	ASN
3	A	158	ASN
3	A	217	ASN
3	A	333	GLN
3	A	389	GLN
3	A	493	GLN
3	A	761	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	GOL	A	1100	-	5,5,5	2.92	1 (20%)	5,5,5	2.34	4 (80%)
7	GOL	A	1101	-	5,5,5	3.05	1 (20%)	5,5,5	2.25	3 (60%)
7	GOL	A	1102	-	5,5,5	2.95	1 (20%)	5,5,5	2.18	2 (40%)
6	TTP	A	1010	4	26,30,30	1.73	6 (23%)	39,47,47	1.26	4 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GOL	A	1100	-	-	2/4/4/4	-
7	GOL	A	1101	-	-	2/4/4/4	-
7	GOL	A	1102	-	-	3/4/4/4	-
6	TTP	A	1010	4	-	3/22/34/34	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1101	GOL	O2-C2	-6.80	1.23	1.43
7	A	1102	GOL	O2-C2	-6.58	1.23	1.43
7	A	1100	GOL	O2-C2	-6.51	1.24	1.43
6	A	1010	TTP	PG-O1G	-3.50	1.39	1.50
6	A	1010	TTP	C6-N1	3.31	1.43	1.38
6	A	1010	TTP	C1'-N1	2.77	1.55	1.48
6	A	1010	TTP	PA-O2A	-2.68	1.42	1.55
6	A	1010	TTP	PB-O1B	-2.54	1.41	1.50
6	A	1010	TTP	PB-O2B	-2.35	1.44	1.55

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1010	TTP	C6-C5-C4	-3.03	115.50	118.03
6	A	1010	TTP	O4'-C1'-N1	2.92	113.08	107.86
7	A	1101	GOL	O2-C2-C1	2.69	120.98	109.12
7	A	1100	GOL	O2-C2-C3	2.68	120.93	109.12
7	A	1102	GOL	O2-C2-C1	2.67	120.88	109.12
7	A	1102	GOL	O2-C2-C3	2.62	120.68	109.12
7	A	1100	GOL	O2-C2-C1	2.62	120.65	109.12
7	A	1101	GOL	O2-C2-C3	2.53	120.26	109.12
7	A	1100	GOL	O1-C1-C2	2.31	121.28	110.20
6	A	1010	TTP	C5M-C5-C4	2.31	121.31	118.77
7	A	1100	GOL	O3-C3-C2	2.24	120.94	110.20
7	A	1101	GOL	O1-C1-C2	2.13	120.42	110.20
6	A	1010	TTP	C5-C4-N3	2.09	117.10	115.31

There are no chirality outliers.

All (10) torsion outliers are listed below:

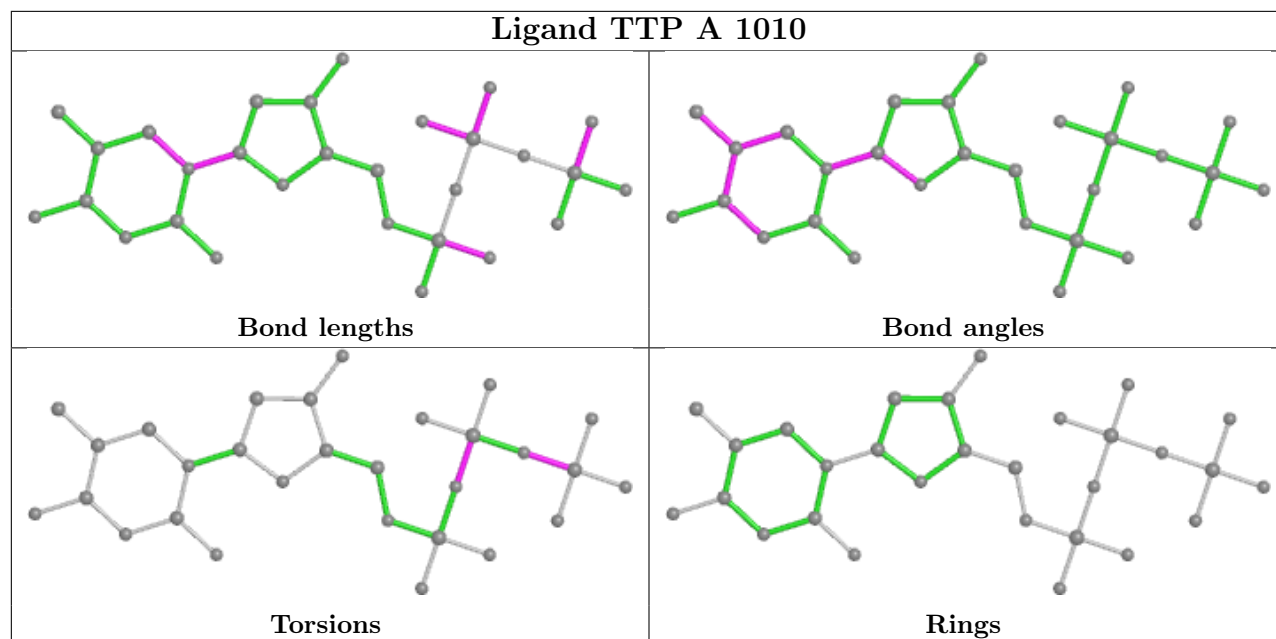
Mol	Chain	Res	Type	Atoms
7	A	1100	GOL	O1-C1-C2-C3
7	A	1101	GOL	O1-C1-C2-C3
7	A	1101	GOL	C1-C2-C3-O3
7	A	1100	GOL	O2-C2-C3-O3
7	A	1102	GOL	O1-C1-C2-C3
7	A	1102	GOL	O1-C1-C2-O2
7	A	1102	GOL	O2-C2-C3-O3
6	A	1010	TTP	PB-O3B-PG-O1G
6	A	1010	TTP	PA-O3A-PB-O2B
6	A	1010	TTP	PB-O3B-PG-O2G

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1100	GOL	1	0
7	A	1101	GOL	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	T	18/18 (100%)	-0.18	1 (5%) 24 25	28, 43, 79, 106	0
2	P	14/14 (100%)	-0.14	0 100 100	27, 45, 76, 82	0
3	A	902/903 (99%)	-0.01	22 (2%) 59 62	22, 45, 77, 103	0
All	All	934/935 (99%)	-0.02	23 (2%) 57 61	22, 45, 77, 106	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	257	TYR	4.7
3	A	44	SER	4.2
3	A	819	ILE	4.1
3	A	258	GLY	3.7
3	A	611	THR	3.4
1	T	1	DA	3.3
3	A	640	LYS	3.2
3	A	793	VAL	2.6
3	A	254	GLU	2.6
3	A	252	VAL	2.5
3	A	817	GLY	2.3
3	A	895	ALA	2.3
3	A	156	TYR	2.3
3	A	311	LYS	2.2
3	A	585	ALA	2.2
3	A	639	SER	2.2
3	A	157	GLY	2.1
3	A	423	VAL	2.1
3	A	589	PHE	2.1
3	A	306	ASP	2.0
3	A	637	GLY	2.0
3	A	816	LYS	2.0
3	A	818	ASN	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](#)

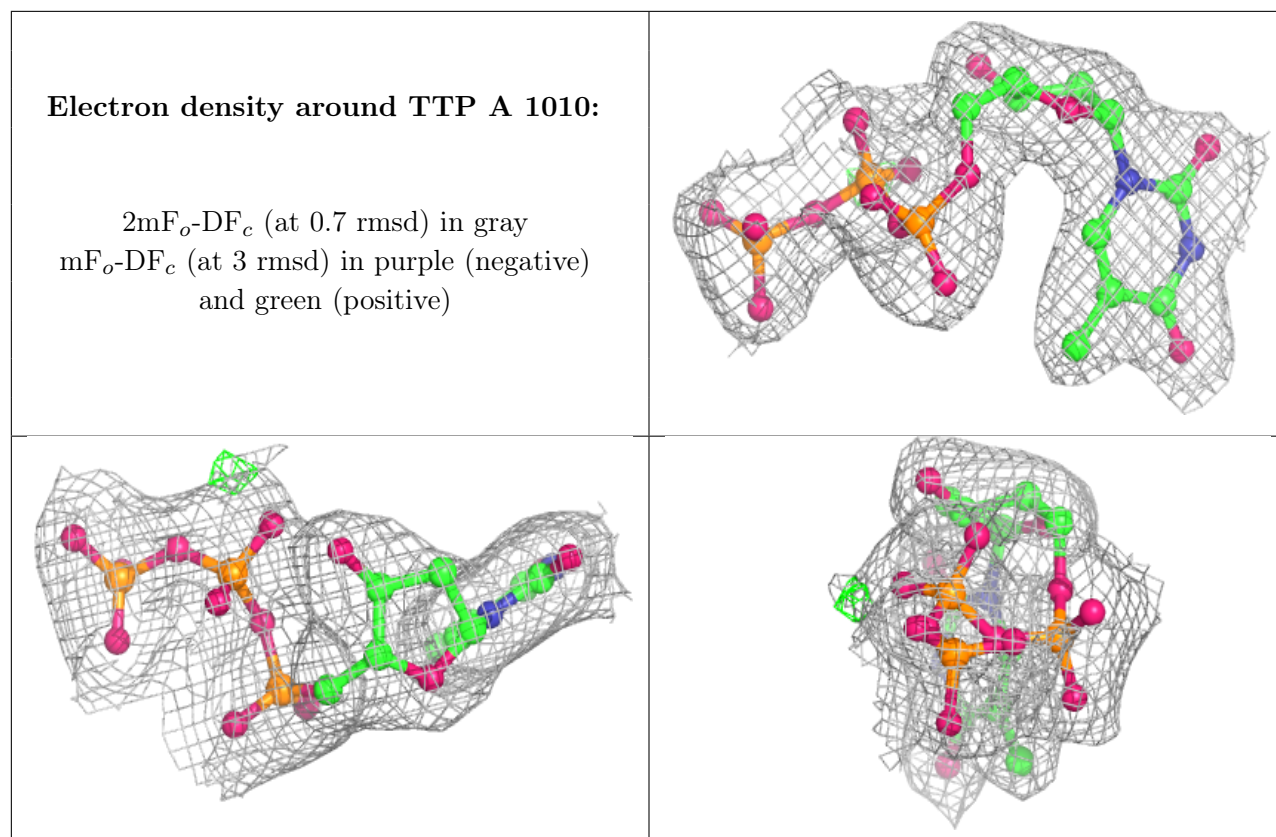
There are no monosaccharides in this entry.

## 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<sup>th</sup> 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	CA	A	1002	1/1	0.59	0.24	87,87,87,87	0
4	CA	A	1006	1/1	0.71	0.07	70,70,70,70	0
5	NA	A	1007	1/1	0.77	0.11	45,45,45,45	0
7	GOL	A	1100	6/6	0.87	0.22	39,45,46,46	0
7	GOL	A	1102	6/6	0.89	0.15	41,49,50,51	0
7	GOL	A	1101	6/6	0.92	0.18	43,44,45,45	0
5	NA	A	1008	1/1	0.93	0.15	67,67,67,67	0
4	CA	A	1005	1/1	0.93	0.13	72,72,72,72	0
4	CA	A	1003	1/1	0.95	0.08	55,55,55,55	0
5	NA	A	1009	1/1	0.96	0.21	56,56,56,56	0
4	CA	A	1004	1/1	0.96	0.05	56,56,56,56	0
6	TTP	A	1010	29/29	0.98	0.13	18,30,36,38	0
4	CA	A	1001	1/1	0.98	0.10	35,35,35,35	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.