



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 10:17 PM BST

PDB ID : 5N2G  
Title : Structure of the E9 DNA polymerase from vaccinia virus in complex with manganese  
Authors : Tarbouriech, N.; Burmeister, W.P.; Iseni, F.  
Deposited on : 2017-02-07  
Resolution : 2.78 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.

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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 : 2.13.1  
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) : 2.13.1

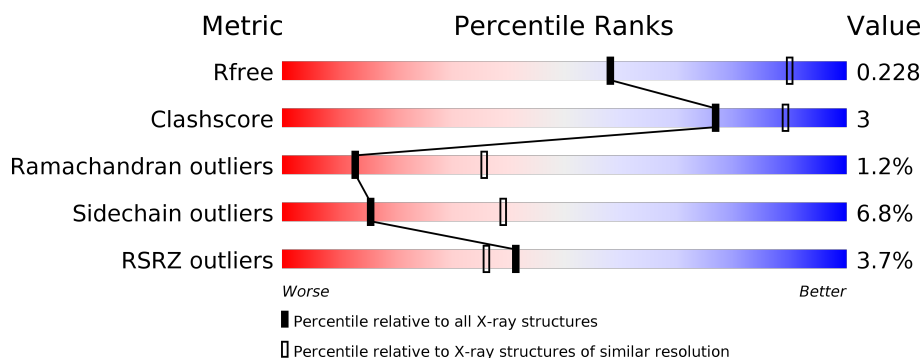
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.78 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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	A	1009	<div> <div>4%</div> <div>87%</div> <div>10% ..</div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8470 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.

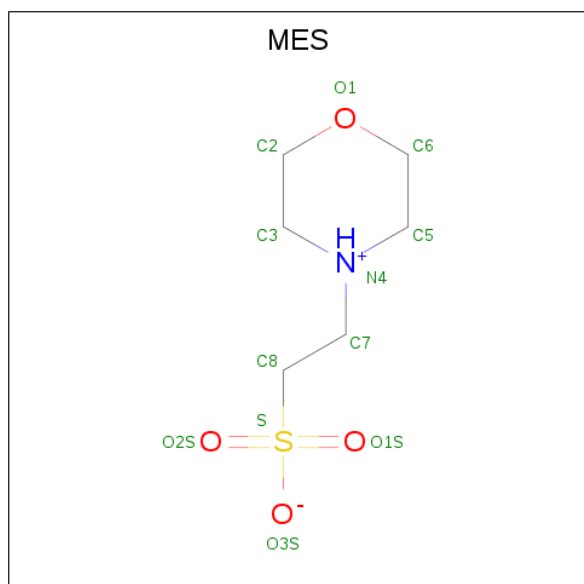
- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	999	8180	5231	1364	1533	52	0	1	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P20509
A	-2	ALA	-	expression tag	UNP P20509
A	-1	MET	-	expression tag	UNP P20509
A	0	ASP	-	expression tag	UNP P20509
A	1	PRO	-	expression tag	UNP P20509

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).

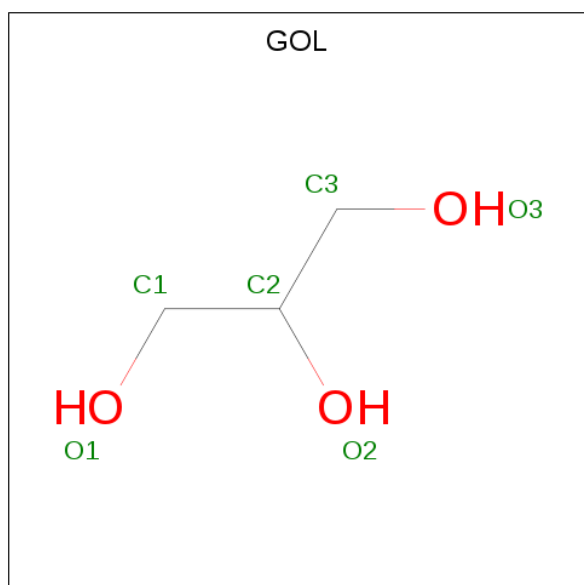


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mn	0	0
			4	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



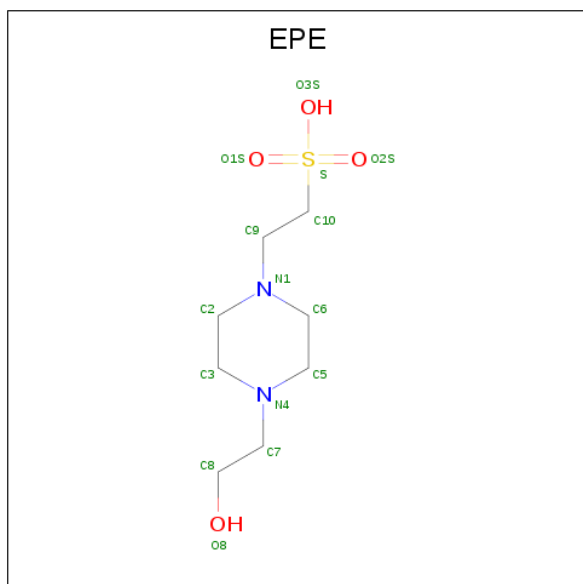
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			8	4	2	2		

- Molecule 6 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

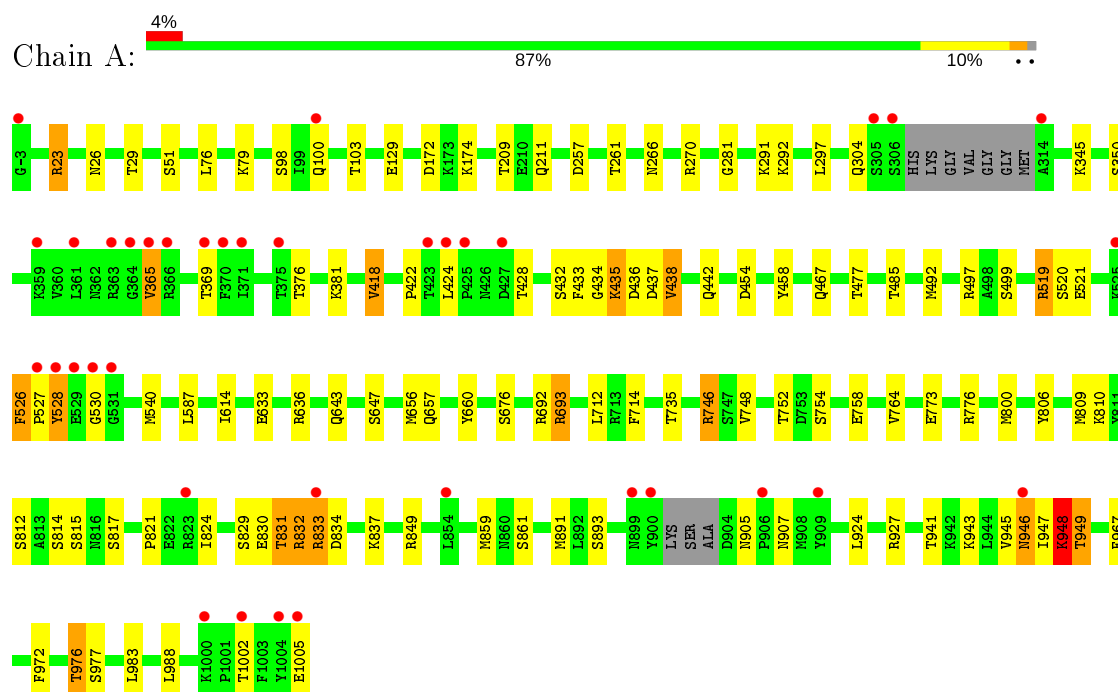
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	215	Total 215	O 215	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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	134.01Å 134.01Å 230.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.78 46.28 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.00-2.78) 98.9 (46.28-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.183 , 0.227 0.188 , 0.228	Depositor DCC
$R_{free}$ test set	2911 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 38.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, GOL, MN, MES, DTT

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	0.57	0/8360	0.80	3/11292 (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	A	0	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	946	ASN	N-CA-C	-6.43	93.64	111.00
1	A	23	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	365	VAL	CB-CA-C	5.28	121.42	111.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	GLY	Peptide
1	A	435	LYS	Peptide
1	A	859	MET	Peptide

## 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	8180	0	8130	49	0
2	A	36	0	39	1	0
3	A	4	0	0	0	0
4	A	12	0	16	0	0
5	A	8	0	10	0	0
6	A	15	0	18	0	0
7	A	215	0	0	6	1
All	All	8470	0	8213	49	1

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 3.

All (49) 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:907:ASN:OD1	1:A:948:LYS:NZ	1.57	1.34
1:A:833:ARG:CG	1:A:893:SER:OG	1.81	1.27
1:A:833:ARG:HB3	1:A:893:SER:N	1.60	1.15
1:A:833:ARG:CB	1:A:893:SER:H	1.67	1.07
1:A:833:ARG:HG3	1:A:893:SER:CB	1.85	1.04
1:A:833:ARG:HG3	1:A:893:SER:OG	0.86	1.02
1:A:833:ARG:HB3	1:A:893:SER:H	0.86	1.00
1:A:945:VAL:HG23	1:A:946:ASN:O	1.81	0.80
1:A:833:ARG:CB	1:A:893:SER:N	2.39	0.70
1:A:519:ARG:NH1	7:A:1201:HOH:O	1.59	0.68
1:A:833:ARG:CG	1:A:893:SER:CB	2.62	0.66
1:A:454:ASP:O	1:A:458[B]:TYR:HD1	1.80	0.63
1:A:442:GLN:HG2	1:A:924:LEU:HD23	1.81	0.62
1:A:454:ASP:O	1:A:458[B]:TYR:CD1	2.53	0.61
1:A:23:ARG:NH1	1:A:29:THR:OG1	2.33	0.61
1:A:712:LEU:HD23	1:A:714:PHE:CZ	2.36	0.60
1:A:587:LEU:HD21	1:A:614:ILE:HD11	1.85	0.59
1:A:773:GLU:OE2	1:A:776:ARG:NH1	2.35	0.59
1:A:350:SER:CB	1:A:434:GLY:HA2	2.33	0.58
1:A:633:GLU:OE2	1:A:636:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:HB2	1:A:434:GLY:HA2	1.88	0.55
1:A:23:ARG:NH2	1:A:257:ASP:OD2	2.41	0.54
1:A:947:ILE:O	1:A:949:THR:N	2.40	0.54
1:A:656:MET:HE3	7:A:1304:HOH:O	2.07	0.53
1:A:972:PHE:O	1:A:976:THR:HG23	2.09	0.53
1:A:266:ASN:OD1	1:A:270:ARG:NH1	2.42	0.52
1:A:643:GLN:NE2	7:A:1202:HOH:O	2.36	0.51
1:A:764:VAL:CG2	1:A:817:SER:HA	2.42	0.50
1:A:633:GLU:HG2	1:A:660:TYR:CZ	2.47	0.49
1:A:76:LEU:HD21	1:A:587:LEU:HA	1.95	0.47
1:A:519:ARG:HD3	7:A:1201:HOH:O	2.14	0.47
1:A:833:ARG:CB	1:A:893:SER:CB	2.93	0.47
1:A:746:ARG:NH1	1:A:758:GLU:OE1	2.45	0.46
1:A:297:LEU:HD23	1:A:297:LEU:C	2.35	0.46
1:A:26:ASN:N	1:A:26:ASN:OD1	2.49	0.46
1:A:810:LYS:HD3	1:A:824:ILE:HD11	2.00	0.43
1:A:209:THR:HG22	1:A:211:GLN:H	1.83	0.43
1:A:947:ILE:C	1:A:949:THR:N	2.72	0.43
1:A:693:ARG:NH1	7:A:1204:HOH:O	2.48	0.42
1:A:369:THR:HG23	1:A:418:VAL:HG12	2.02	0.42
1:A:812:SER:O	1:A:815:SER:HB3	2.19	0.42
1:A:800:MET:HB2	1:A:806:TYR:HB2	2.02	0.42
1:A:831:THR:HG22	1:A:832:ARG:H	1.86	0.41
1:A:485:THR:HG23	1:A:660:TYR:CZ	2.56	0.41
1:A:647:SER:HB3	7:A:1388:HOH:O	2.20	0.41
1:A:587:LEU:HD21	1:A:614:ILE:CD1	2.49	0.41
1:A:436:ASP:HB2	1:A:458[B]:TYR:CD2	2.57	0.40
1:A:438:VAL:HG13	1:A:458[B]:TYR:HE2	1.87	0.40
1:A:497:ARG:HG2	2:A:1102:MES:O1S	2.21	0.40

All (1) 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)
7:A:1221:HOH:O	7:A:1221:HOH:O[6_555]	0.62	1.58

## 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	994/1009 (98%)	939 (94%)	43 (4%)	12 (1%)	13	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	PRO
1	A	435	LYS
1	A	527	PRO
1	A	528	TYR
1	A	948	LYS
1	A	821	PRO
1	A	832	ARG
1	A	830	GLU
1	A	365	VAL
1	A	943	LYS
1	A	526	PHE
1	A	530	GLY

### 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	923/928 (100%)	860 (93%)	63 (7%)	16	39

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER
1	A	79	LYS
1	A	98	SER
1	A	100	GLN
1	A	103	THR
1	A	129	GLU
1	A	172	ASP
1	A	174	LYS
1	A	261	THR
1	A	291	LYS
1	A	292	LYS
1	A	304	GLN
1	A	345	LYS
1	A	376	THR
1	A	381	LYS
1	A	418	VAL
1	A	424	LEU
1	A	428	THR
1	A	432	SER
1	A	433	PHE
1	A	437	ASP
1	A	438	VAL
1	A	467	GLN
1	A	477	THR
1	A	492	MET
1	A	499	SER
1	A	519	ARG
1	A	520	SER
1	A	521	GLU
1	A	526	PHE
1	A	528	TYR
1	A	540	MET
1	A	657	GLN
1	A	676	SER
1	A	692	ARG
1	A	693	ARG
1	A	735	THR
1	A	746	ARG
1	A	748	VAL
1	A	752	THR
1	A	754	SER
1	A	809	MET
1	A	814	SER

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Mol	Chain	Res	Type
1	A	829	SER
1	A	831	THR
1	A	833	ARG
1	A	834	ASP
1	A	837	LYS
1	A	849	ARG
1	A	861	SER
1	A	891	MET
1	A	905	ASN
1	A	927	ARG
1	A	941	THR
1	A	948	LYS
1	A	949	THR
1	A	967	PHE
1	A	976	THR
1	A	977	SER
1	A	983	LEU
1	A	988	LEU
1	A	1002	THR
1	A	1005	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	839	HIS
1	A	897	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	DTT	A	1110	-	7,7,7	0.90	0	4,8,8	0.86	0
2	MES	A	1102	-	12,12,12	1.92	1 (8%)	14,16,16	2.01	4 (28%)
6	EPE	A	1111	-	15,15,15	2.04	1 (6%)	18,20,20	1.54	3 (16%)
2	MES	A	1103	-	12,12,12	2.01	1 (8%)	14,16,16	2.65	5 (35%)
4	GOL	A	1109	-	5,5,5	0.33	0	5,5,5	0.83	0
4	GOL	A	1108	-	5,5,5	0.47	0	5,5,5	0.45	0
2	MES	A	1101	-	12,12,12	2.09	1 (8%)	14,16,16	2.19	5 (35%)

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	DTT	A	1110	-	-	6/8/8/8	-
2	MES	A	1102	-	-	3/6/14/14	0/1/1/1
6	EPE	A	1111	-	-	4/9/19/19	0/1/1/1
2	MES	A	1103	-	-	4/6/14/14	0/1/1/1
4	GOL	A	1109	-	-	0/4/4/4	-
4	GOL	A	1108	-	-	1/4/4/4	-
2	MES	A	1101	-	-	0/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1111	EPE	C10-S	-7.38	1.67	1.77
2	A	1101	MES	C8-S	-6.85	1.67	1.77
2	A	1103	MES	C8-S	-6.18	1.68	1.77
2	A	1102	MES	C8-S	-6.17	1.68	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	MES	O3S-S-C8	5.57	114.78	105.77
2	A	1102	MES	O2S-S-C8	5.16	113.12	106.92
2	A	1101	MES	O3S-S-C8	5.15	114.11	105.77
2	A	1103	MES	O1S-S-C8	4.69	112.57	106.92
2	A	1103	MES	C6-C5-N4	4.65	117.16	110.10
6	A	1111	EPE	O3S-S-C10	4.43	112.93	105.77
2	A	1101	MES	O2S-S-C8	-3.65	102.53	106.92
2	A	1102	MES	O3S-S-C8	3.60	111.58	105.77
2	A	1103	MES	C2-C3-N4	3.21	114.97	110.10
2	A	1101	MES	O1S-S-C8	2.91	110.42	106.92
6	A	1111	EPE	O3S-S-O2S	-2.60	104.92	111.27
2	A	1101	MES	O1-C2-C3	-2.43	106.45	111.80
2	A	1103	MES	O3S-S-O1S	-2.39	105.43	111.27
2	A	1102	MES	O3S-S-O2S	-2.19	105.93	111.27
2	A	1101	MES	C7-N4-C3	-2.18	105.66	111.23
2	A	1102	MES	O2S-S-O1S	-2.12	106.59	113.95
6	A	1111	EPE	O2S-S-C10	2.05	109.38	106.92

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1110	DTT	S1-C1-C2-O2
5	A	1110	DTT	S1-C1-C2-C3
5	A	1110	DTT	C1-C2-C3-O3
5	A	1110	DTT	C1-C2-C3-C4
5	A	1110	DTT	O2-C2-C3-O3
5	A	1110	DTT	O2-C2-C3-C4
2	A	1102	MES	C7-C8-S-O1S
2	A	1102	MES	C7-C8-S-O2S
2	A	1102	MES	C7-C8-S-O3S
6	A	1111	EPE	C9-C10-S-O1S
2	A	1103	MES	C7-C8-S-O2S
6	A	1111	EPE	C9-C10-S-O3S
6	A	1111	EPE	N4-C7-C8-O8
2	A	1103	MES	C7-C8-S-O1S
2	A	1103	MES	C7-C8-S-O3S
2	A	1103	MES	N4-C7-C8-S
4	A	1108	GOL	C1-C2-C3-O3
6	A	1111	EPE	C9-C10-S-O2S



There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1102	MES	1	0

## 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	A	999/1009 (99%)	0.02	37 (3%) 41 36	36, 65, 127, 172	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	531	GLY	5.6
1	A	528	TYR	4.4
1	A	527	PRO	4.1
1	A	366	ARG	4.0
1	A	900	TYR	3.8
1	A	364	GLY	3.8
1	A	365	VAL	3.6
1	A	899	ASN	3.5
1	A	359	LYS	3.5
1	A	371	ILE	3.3
1	A	423	THR	3.3
1	A	1002	THR	3.1
1	A	305	SER	3.0
1	A	306	SER	3.0
1	A	424	LEU	3.0
1	A	361	LEU	2.9
1	A	314	ALA	2.9
1	A	370	PHE	2.8
1	A	1004	TYR	2.7
1	A	425	PRO	2.7
1	A	906	PRO	2.7
1	A	833	ARG	2.7
1	A	823	ARG	2.7
1	A	427	ASP	2.7
1	A	909	TYR	2.7
1	A	530	GLY	2.6
1	A	946	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	529	GLU	2.5
1	A	1000	LYS	2.4
1	A	854	LEU	2.3
1	A	525	LYS	2.2
1	A	375	THR	2.2
1	A	363	ARG	2.2
1	A	-3	GLY	2.2
1	A	369	THR	2.2
1	A	100	GLN	2.1
1	A	1005	GLU	2.1

## 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	GOL	A	1108	6/6	0.73	0.27	102,114,115,116	0
6	EPE	A	1111	15/15	0.83	0.33	101,113,120,126	0
5	DTT	A	1110	8/8	0.84	0.30	110,128,135,136	0
2	MES	A	1103	12/12	0.89	0.38	121,126,146,149	0
4	GOL	A	1109	6/6	0.91	0.28	74,75,78,85	0
2	MES	A	1101	12/12	0.95	0.17	66,70,74,75	0
3	MN	A	1106	1/1	0.96	0.21	74,74,74,74	1
2	MES	A	1102	12/12	0.97	0.15	73,83,87,87	0
3	MN	A	1104	1/1	0.98	0.20	76,76,76,76	0
3	MN	A	1105	1/1	0.99	0.27	53,53,53,53	0
3	MN	A	1107	1/1	0.99	0.17	86,86,86,86	0

## 6.5 Other polymers

There are no such residues in this entry.