



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:44 AM UTC

PDB ID : 5N2G / pdb_00005n2g
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

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
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

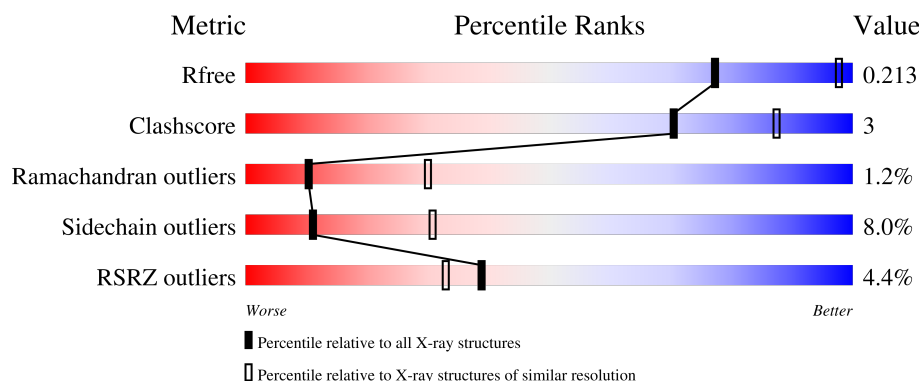
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (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 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	1009	

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.

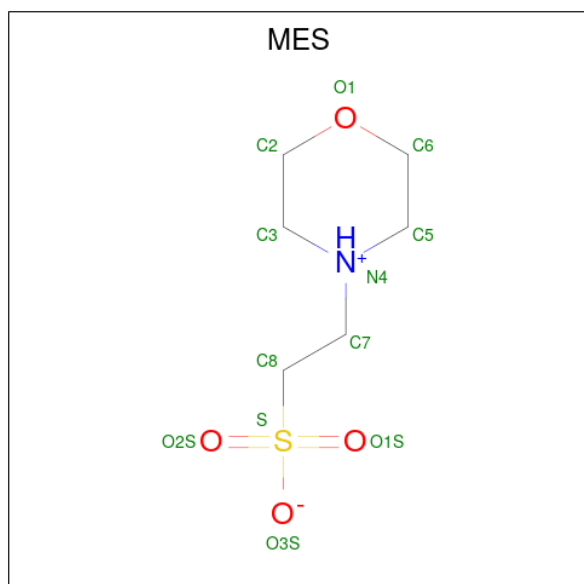
- Molecule 1 is a protein called DNA polymerase.

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 (CCD ID: MES) (formula: C₆H₁₃NO₄S).

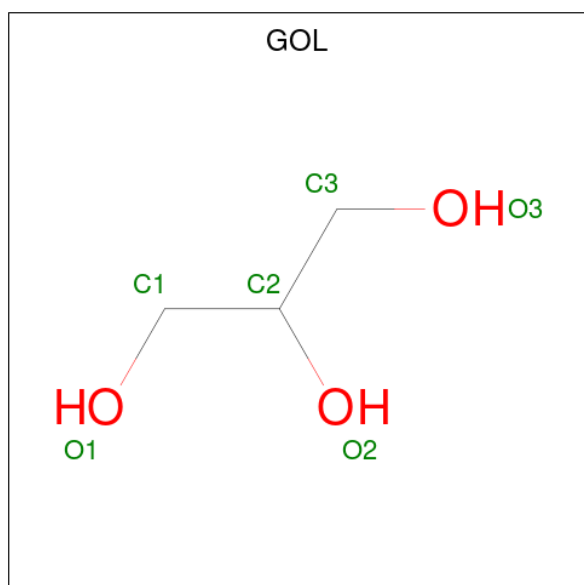


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

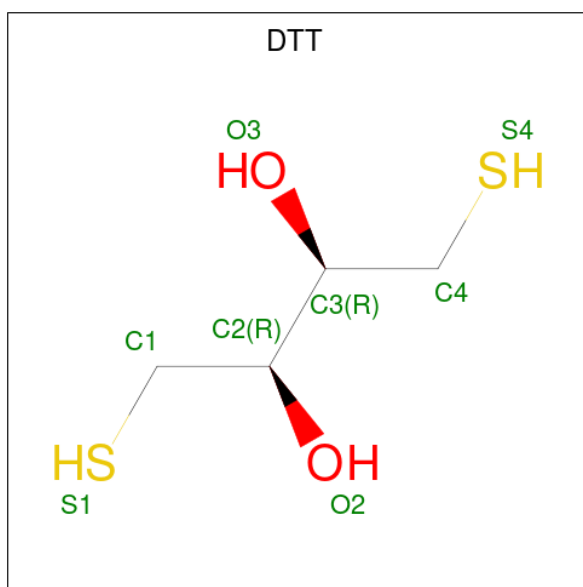
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mn	0	0
			4	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



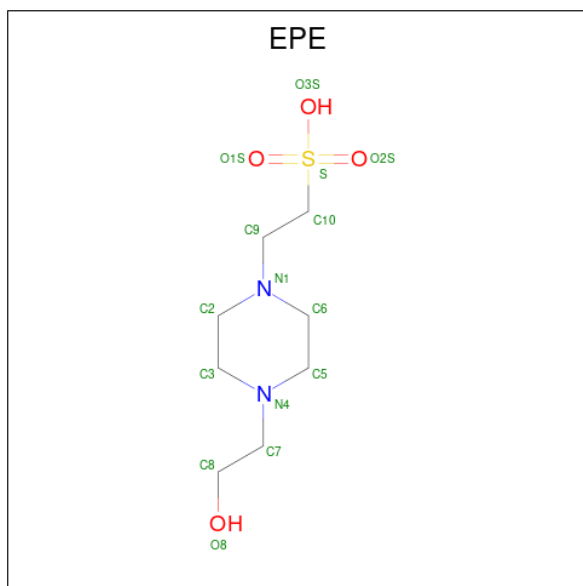
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



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 (CCD ID: 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, α , β , γ	134.01Å 134.01Å 230.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.00 – 2.78 46.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.3 (46.00-2.78) 98.8 (46.00-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.183 , 0.227 (Not available) , 0.213	Depositor DCC
R_{free} test set	2911 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	64.2	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: MES, DTT, MN, EPE, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.77	0/8360	0.98	6/11292 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	834	ASP	N-CA-C	-12.88	98.04	113.88
1	A	946	ASN	N-CA-C	-10.85	93.64	109.59
1	A	862	ASN	N-CA-C	8.19	120.28	111.36
1	A	365	VAL	CB-CA-C	6.18	121.42	111.29
1	A	315	ASN	N-CA-C	6.09	118.39	110.53
1	A	945	VAL	O-C-N	5.28	129.17	122.57

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	56	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	56	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 (56) 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:HG3	1:A:893:SER:HG	1.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:TYR:OH	1:A:455:MET:HE1	2.06	0.56
1:A:633:GLU:OE2	1:A:636:ARG:NH1	2.39	0.56
1:A:350:SER:HB2	1:A:434:GLY:HA2	1.88	0.55
1:A:8:TRP:CG	1:A:114:TYR:HH	2.25	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: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:297:LEU:C	1:A:297:LEU:HD23	2.35	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:656:MET:HE3	7:A:1304:HOH:O	2.12	0.49
1:A:76:LEU:HD21	1:A:587:LEU:HA	1.95	0.47
1:A:947:ILE:C	1:A:949:THR:N	2.72	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:26:ASN:OD1	1:A:26:ASN:N	2.49	0.46
1:A:765:ASP:CG	1:A:817:SER:HB2	2.43	0.44
1:A:947:ILE:C	1:A:949:THR:H	2.26	0.44
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: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:455:MET:HB3	1:A:455:MET:HE2	1.87	0.41
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:227:LEU:C	1:A:227:LEU:HD23	2.46	0.40
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%)	10 30

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%)	849 (92%)	74 (8%)	11	31

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	26	ASN
1	A	43	THR
1	A	51	SER
1	A	79	LYS
1	A	95	LYS
1	A	98	SER
1	A	100	GLN
1	A	103	THR
1	A	129	GLU
1	A	172	ASP
1	A	173	LYS
1	A	174	LYS
1	A	215	GLU
1	A	228	MET
1	A	261	THR
1	A	277	GLU
1	A	278	LEU
1	A	291	LYS
1	A	292	LYS
1	A	304	GLN
1	A	340	LYS
1	A	345	LYS
1	A	376	THR
1	A	381	LYS
1	A	418	VAL
1	A	420	LEU
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	499	SER
1	A	520	SER
1	A	521	GLU

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Mol	Chain	Res	Type
1	A	526	PHE
1	A	540	MET
1	A	587	LEU
1	A	633	GLU
1	A	676	SER
1	A	693	ARG
1	A	701	VAL
1	A	735	THR
1	A	748	VAL
1	A	752	THR
1	A	754	SER
1	A	800	MET
1	A	809	MET
1	A	814	SER
1	A	829	SER
1	A	831	THR
1	A	834	ASP
1	A	835	VAL
1	A	837	LYS
1	A	849	ARG
1	A	864	VAL
1	A	873	GLU
1	A	891	MET
1	A	905	ASN
1	A	927	ARG
1	A	941	THR
1	A	947	ILE
1	A	948	LYS
1	A	949	THR
1	A	976	THR
1	A	977	SER
1	A	978	GLU
1	A	983	LEU
1	A	988	LEU
1	A	1002	THR
1	A	1005	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	336	GLN

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Mol	Chain	Res	Type
1	A	584	ASN
1	A	600	HIS
1	A	607	ASN
1	A	716	ASN
1	A	839	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	$\# Z > 2$
6	EPE	A	1111	-	15,15,15	2.08	1 (6%)	19,20,20	1.36	3 (15%)
2	MES	A	1102	-	12,12,12	1.97	1 (8%)	15,16,16	1.71	4 (26%)
4	GOL	A	1108	-	5,5,5	0.49	0	5,5,5	0.47	0
5	DTT	A	1110	-	7,7,7	0.91	0	4,8,8	0.89	0
4	GOL	A	1109	-	5,5,5	0.34	0	5,5,5	0.91	0
2	MES	A	1103	-	12,12,12	2.06	1 (8%)	15,16,16	2.30	5 (33%)
2	MES	A	1101	-	12,12,12	2.14	1 (8%)	15,16,16	1.83	5 (33%)

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
6	EPE	A	1111	-	-	4/9/19/19	0/1/1/1
2	MES	A	1102	-	-	3/6/14/14	0/1/1/1
4	GOL	A	1108	-	-	1/4/4/4	-
5	DTT	A	1110	-	-	6/8/8/8	-
4	GOL	A	1109	-	-	0/4/4/4	-
2	MES	A	1103	-	-	3/6/14/14	0/1/1/1
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	-7.54	1.67	1.77
2	A	1101	MES	C8-S	-7.00	1.67	1.77
2	A	1103	MES	C8-S	-6.33	1.68	1.77
2	A	1102	MES	C8-S	-6.31	1.68	1.77

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	MES	C6-C5-N4	4.63	117.16	110.12
2	A	1103	MES	O3S-S-C8	4.48	114.78	106.00
2	A	1102	MES	O2S-S-C8	4.23	113.12	106.73
2	A	1101	MES	O3S-S-C8	4.14	114.11	106.00
2	A	1103	MES	O1S-S-C8	3.86	112.57	106.73
6	A	1111	EPE	O3S-S-C10	3.54	112.93	106.00
2	A	1103	MES	C2-C3-N4	3.19	114.97	110.12
2	A	1102	MES	O3S-S-C8	2.85	111.58	106.00
2	A	1101	MES	O2S-S-C8	-2.78	102.53	106.73
6	A	1111	EPE	O3S-S-O2S	-2.59	104.92	111.40
2	A	1101	MES	O1-C2-C3	-2.47	106.45	111.77
2	A	1101	MES	O1S-S-C8	2.44	110.42	106.73
2	A	1103	MES	O3S-S-O1S	-2.39	105.43	111.40
2	A	1102	MES	O2S-S-O1S	-2.22	106.59	113.82
2	A	1102	MES	O3S-S-O2S	-2.19	105.93	111.40
2	A	1101	MES	C7-N4-C3	-2.09	105.66	111.24
6	A	1111	EPE	C6-N1-C2	2.08	113.31	108.84

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1102	MES	C7-C8-S-O1S
2	A	1102	MES	C7-C8-S-O2S
2	A	1102	MES	C7-C8-S-O3S
2	A	1103	MES	C7-C8-S-O2S
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
6	A	1111	EPE	C9-C10-S-O1S
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
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, 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	999/1009 (99%)	-0.06	44 (4%)	39 33	30, 65, 127, 172	1 (0%)

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	PRO	5.5
1	A	900	TYR	4.7
1	A	306	SER	4.4
1	A	528	TYR	4.3
1	A	424	LEU	4.2
1	A	944	LEU	4.2
1	A	532	LYS	3.8
1	A	1004	TYR	3.4
1	A	831	THR	3.3
1	A	423	THR	3.2
1	A	175	PHE	3.2
1	A	832	ARG	3.1
1	A	314	ALA	3.0
1	A	365	VAL	3.0
1	A	526	PHE	2.9
1	A	534	PHE	2.9
1	A	174	LYS	2.7
1	A	948	LYS	2.7
1	A	945	VAL	2.5
1	A	420	LEU	2.5
1	A	437	ASP	2.5
1	A	435	LYS	2.4
1	A	829	SER	2.4
1	A	533	VAL	2.4
1	A	95	LYS	2.3
1	A	947	ILE	2.3
1	A	1002	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	525	LYS	2.3
1	A	436	ASP	2.3
1	A	833	ARG	2.3
1	A	531	GLY	2.3
1	A	361	LEU	2.2
1	A	79	LYS	2.2
1	A	100	GLN	2.2
1	A	809	MET	2.2
1	A	828	THR	2.2
1	A	378	ALA	2.1
1	A	956	ARG	2.1
1	A	987	VAL	2.1
1	A	180	ILE	2.1
1	A	380	GLY	2.1
1	A	908	MET	2.1
1	A	434	GLY	2.0
1	A	899	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 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
6	EPE	A	1111	15/15	0.81	0.25	101,113,120,126	0
4	GOL	A	1108	6/6	0.86	0.21	102,114,115,116	0
5	DTT	A	1110	8/8	0.88	0.19	110,128,135,136	0
2	MES	A	1103	12/12	0.90	0.25	121,126,146,149	0
4	GOL	A	1109	6/6	0.91	0.18	74,75,78,85	0
2	MES	A	1102	12/12	0.94	0.14	73,83,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	1101	12/12	0.95	0.12	66,70,74,75	0
3	MN	A	1106	1/1	0.98	0.08	74,74,74,74	1
3	MN	A	1107	1/1	0.98	0.06	86,86,86,86	0
3	MN	A	1105	1/1	0.98	0.09	53,53,53,53	0
3	MN	A	1104	1/1	0.99	0.03	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.