



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:30 PM UTC

PDB ID : 5N2E / pdb_00005n2e
Title : Structure of the E9 DNA polymerase from vaccinia virus
Authors : Tarbouriech, N.; Burmeister, W.P.; Iseni, F.
Deposited on : 2017-02-07
Resolution : 2.74 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

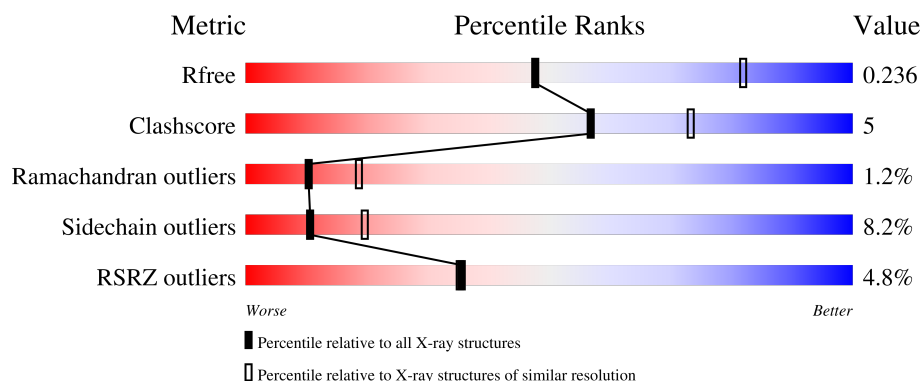
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	1010	5% 83% 13% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8478 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.

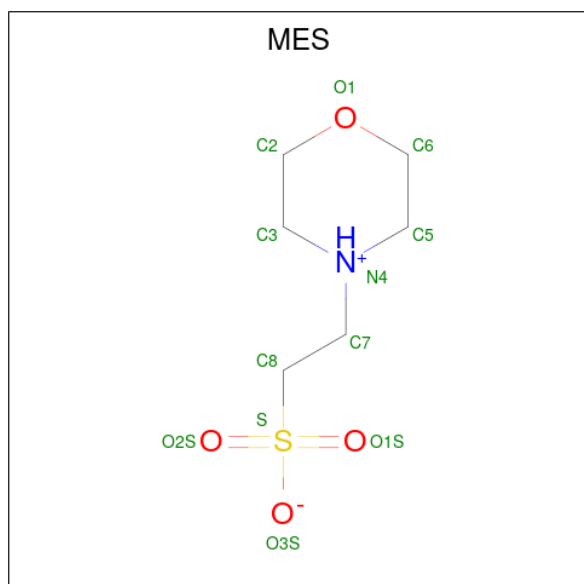
- Molecule 1 is a protein called DNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	999	8188	5239	1364	1533	52	0	2	0

There are 5 discrepancies between the modelled and reference sequences:

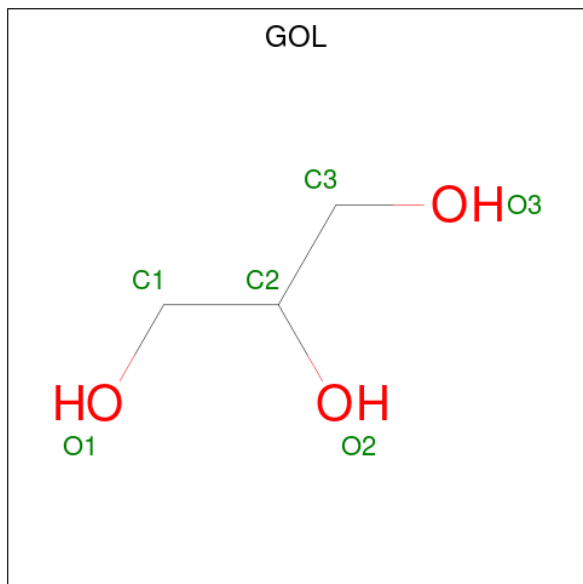
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP P20509
A	-2	ALA	-	expression tag	UNP P20509
A	-1	MET	-	expression tag	UNP P20509
A	0	ASP	-	expression tag	UNP P20509
A	1	PRO	-	expression tag	UNP P20509

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



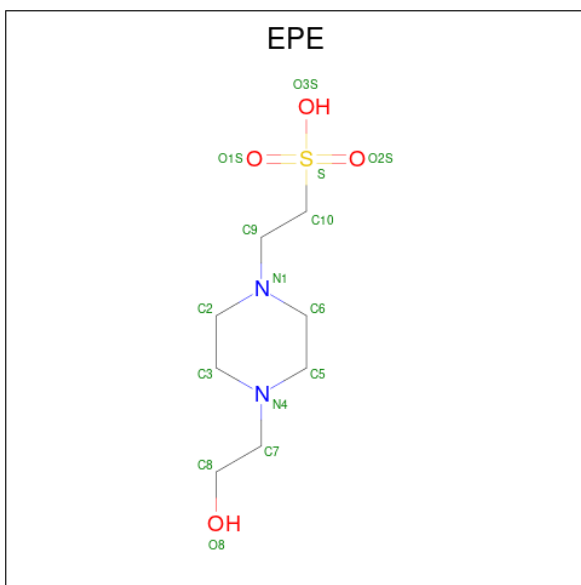
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
2	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



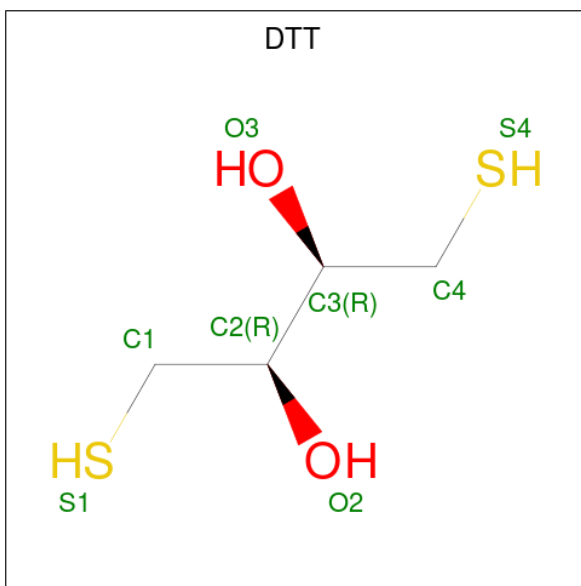
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

- Molecule 5 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: $C_4H_{10}O_2S_2$).



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

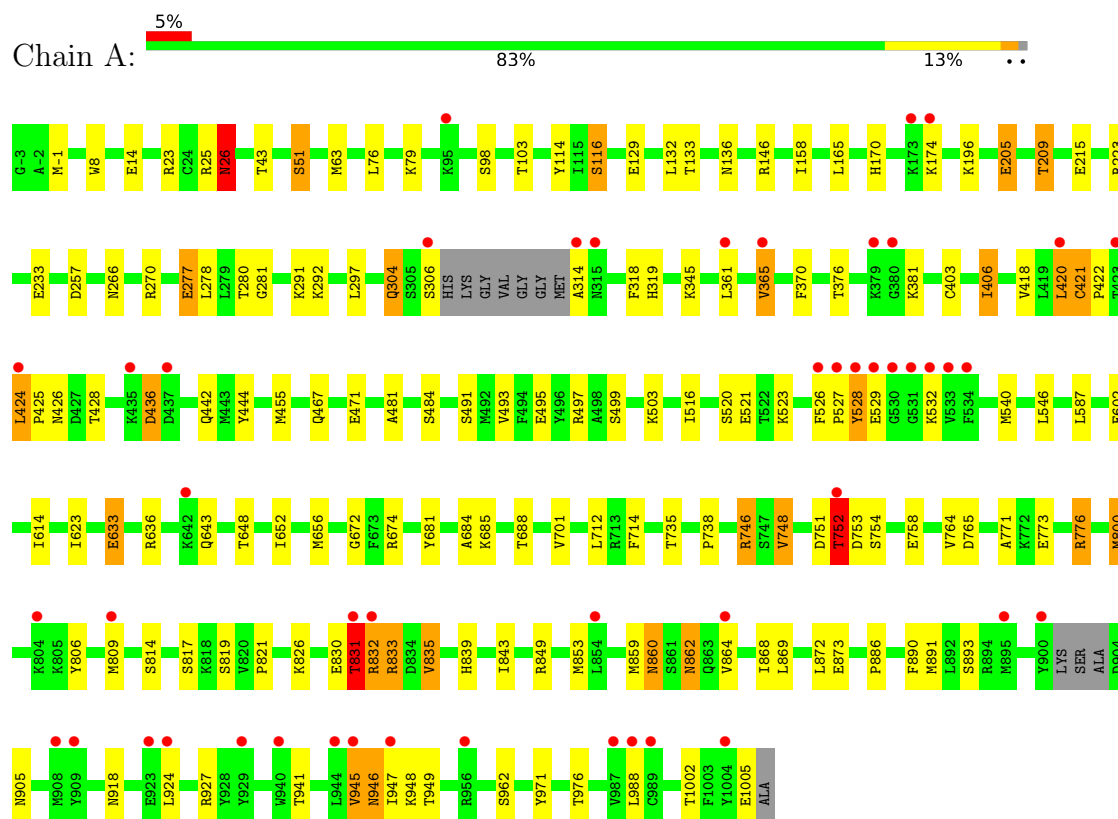
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total 219	O 219	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	133.41Å 133.41Å 230.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	115.81 – 2.74 115.54 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (115.81-2.74) 99.8 (115.54-2.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.186 , 0.236 0.191 , 0.236	Depositor DCC
R_{free} test set	3075 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	64.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8478	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: GOL, EPE, DTT, MES

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	1.02	3/8372 (0.0%)	1.11	15/11309 (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	4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ILE	C-O	-7.66	1.18	1.24
1	A	623	ILE	C-O	-5.23	1.20	1.24
1	A	26	ASN	N-CA	5.15	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	862	ASN	N-CA-C	7.52	122.28	113.18
1	A	365	VAL	CB-CA-C	6.96	122.71	111.29
1	A	205	GLU	CB-CA-C	-6.63	99.73	110.74
1	A	136	ASN	N-CA-C	-6.38	100.12	109.18
1	A	436	ASP	CB-CA-C	6.18	120.31	109.80
1	A	503	LYS	N-CA-C	6.17	118.81	111.71
1	A	471	GLU	N-CA-C	-5.93	104.73	111.14
1	A	748	VAL	CB-CA-C	5.86	116.65	110.91
1	A	421	CYS	CA-C-N	5.58	126.82	119.84
1	A	421	CYS	C-N-CA	5.58	126.82	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	SER	N-CA-C	5.55	118.09	111.71
1	A	471	GLU	N-CA-CB	5.33	117.79	110.07
1	A	860	ASN	N-CA-C	-5.24	101.86	109.31
1	A	946	ASN	N-CA-C	-5.12	99.42	108.23
1	A	493	VAL	CB-CA-C	-5.12	105.42	111.97

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	281	GLY	Peptide
1	A	424	LEU	Peptide
1	A	859	MET	Peptide
1	A	860	ASN	Peptide

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	A	8188	0	8140	76	0
2	A	36	0	39	4	0
3	A	12	0	16	0	0
4	A	15	0	18	0	0
5	A	8	0	10	0	0
6	A	219	0	0	5	1
All	All	8478	0	8223	76	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 5.

All (76) 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:833:ARG:HG3	1:A:893:SER:OG	1.49	1.08
1:A:946:ASN:C	1:A:948:LYS:H	1.92	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:681:TYR:CZ	1:A:685:LYS:HD2	2.25	0.71
1:A:266:ASN:OD1	1:A:270:ARG:NH1	2.29	0.66
1:A:444:TYR:OH	1:A:455:MET:HE1	1.97	0.64
1:A:753:ASP:HB2	6:A:1317:HOH:O	1.98	0.63
1:A:946:ASN:C	1:A:948:LYS:N	2.53	0.63
1:A:528[B]:TYR:CD1	1:A:685:LYS:HG2	2.33	0.62
1:A:833:ARG:CG	1:A:893:SER:OG	2.39	0.61
1:A:833:ARG:HB3	1:A:893:SER:H	1.66	0.59
1:A:495:GLU:OE1	2:A:1103:MES:H52	2.03	0.59
1:A:528[B]:TYR:CE2	1:A:688:THR:HG21	2.39	0.58
1:A:23:ARG:NH2	1:A:257:ASP:OD2	2.37	0.58
1:A:266:ASN:O	1:A:270:ARG:HD2	2.04	0.57
1:A:304:GLN:O	1:A:314:ALA:HB3	2.04	0.57
1:A:63:MET:HE2	1:A:516:ILE:HG13	1.87	0.57
1:A:681:TYR:CE1	1:A:685:LYS:HD2	2.39	0.56
1:A:497:ARG:HG2	2:A:1102:MES:O1S	2.06	0.55
1:A:764:VAL:CG2	1:A:817:SER:HA	2.36	0.55
1:A:528[A]:TYR:CD2	1:A:684:ALA:HB1	2.42	0.55
1:A:751:ASP:O	1:A:752:THR:C	2.50	0.54
1:A:403:CYS:SG	1:A:421:CYS:HB3	2.48	0.53
1:A:833:ARG:HG3	1:A:893:SER:CB	2.36	0.52
1:A:205:GLU:OE2	1:A:223:ARG:NE	2.43	0.52
1:A:546:LEU:HD22	1:A:771:ALA:HB2	1.90	0.52
1:A:8:TRP:CG	1:A:114:TYR:HH	2.28	0.52
1:A:800:MET:HB2	1:A:806:TYR:HB2	1.93	0.51
1:A:862:ASN:N	1:A:862:ASN:OD1	2.44	0.51
1:A:528[A]:TYR:CE2	1:A:672:GLY:HA3	2.44	0.51
1:A:26:ASN:N	1:A:26:ASN:OD1	2.43	0.50
1:A:297:LEU:C	1:A:297:LEU:HD23	2.35	0.50
1:A:712:LEU:HD23	1:A:714:PHE:CZ	2.46	0.50
1:A:495:GLU:OE1	2:A:1103:MES:H61	2.12	0.50
1:A:751:ASP:O	1:A:753:ASP:N	2.44	0.50
1:A:831:THR:O	1:A:832:ARG:C	2.56	0.49
1:A:528[A]:TYR:CE2	1:A:684:ALA:HB1	2.48	0.49
1:A:587:LEU:HD21	1:A:614:ILE:HD11	1.95	0.48
1:A:833:ARG:NH1	1:A:835:VAL:O	2.47	0.48
1:A:481:ALA:HA	1:A:656:MET:HE2	1.96	0.48
1:A:528[B]:TYR:HE2	1:A:688:THR:HG21	1.77	0.48
1:A:890:PHE:HB3	1:A:971:TYR:CZ	2.49	0.47
1:A:656:MET:HE3	6:A:1275:HOH:O	2.13	0.47
1:A:528[B]:TYR:CD1	1:A:685:LYS:CG	2.98	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:SER:HB2	2:A:1103:MES:H21	1.97	0.46
1:A:633:GLU:OE2	1:A:636:ARG:NH1	2.49	0.45
1:A:833:ARG:HB3	1:A:893:SER:N	2.30	0.45
1:A:23:ARG:HH22	1:A:257:ASP:CG	2.24	0.45
1:A:442:GLN:HG2	1:A:924:LEU:CD2	2.47	0.45
1:A:835:VAL:HG13	1:A:839:HIS:HB3	1.98	0.45
1:A:133:THR:HG22	6:A:1396:HOH:O	2.16	0.44
1:A:853:MET:HE3	1:A:864:VAL:HG22	2.00	0.44
1:A:946:ASN:O	1:A:948:LYS:N	2.51	0.44
1:A:444:TYR:CZ	1:A:455:MET:HE1	2.53	0.44
1:A:746:ARG:NH1	1:A:758:GLU:OE1	2.47	0.44
1:A:170:HIS:HA	1:A:444:TYR:CZ	2.52	0.44
1:A:872:LEU:HD21	1:A:976:THR:HG22	1.99	0.44
1:A:266:ASN:HB2	1:A:318:PHE:CD2	2.53	0.43
1:A:170:HIS:HA	1:A:444:TYR:CE2	2.54	0.43
1:A:406:ILE:HD11	1:A:420:LEU:HB2	2.01	0.43
1:A:523:LYS:HE2	1:A:674:ARG:O	2.19	0.42
1:A:800:MET:HB2	1:A:806:TYR:CB	2.49	0.42
1:A:-1:MET:HE1	1:A:132:LEU:CD1	2.49	0.42
1:A:319:HIS:CE1	1:A:495:GLU:HG3	2.55	0.42
1:A:765:ASP:CG	1:A:817:SER:HB2	2.45	0.42
1:A:209:THR:HG21	6:A:1259:HOH:O	2.19	0.41
1:A:681:TYR:CZ	1:A:685:LYS:CD	2.98	0.41
1:A:830:GLU:HG3	1:A:831:THR:N	2.35	0.41
1:A:76:LEU:HD21	1:A:587:LEU:HA	2.03	0.41
1:A:277:GLU:O	1:A:280:THR:O	2.38	0.41
1:A:773:GLU:OE2	1:A:776:ARG:NH1	2.54	0.41
1:A:945:VAL:HB	1:A:946:ASN:H	1.66	0.41
1:A:165:LEU:HD12	1:A:165:LEU:C	2.46	0.41
1:A:918:ASN:HB3	6:A:1285:HOH:O	2.21	0.41
1:A:116:SER:O	1:A:146:ARG:NH1	2.53	0.40
1:A:370:PHE:CD1	1:A:370:PHE:N	2.90	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)
6:A:1265:HOH:O	6:A:1265:HOH:O[6_555]	0.71	1.49

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	995/1010 (98%)	921 (93%)	61 (6%)	13 (1%)	9 16

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	PRO
1	A	527	PRO
1	A	528[A]	TYR
1	A	528[B]	TYR
1	A	752	THR
1	A	821	PRO
1	A	51	SER
1	A	365	VAL
1	A	831	THR
1	A	945	VAL
1	A	832	ARG
1	A	425	PRO
1	A	947	ILE

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	924/928 (100%)	847 (92%)	77 (8%)	10 19

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	25	ARG
1	A	26	ASN
1	A	43	THR
1	A	51	SER
1	A	79	LYS
1	A	98	SER
1	A	103	THR
1	A	129	GLU
1	A	174	LYS
1	A	196	LYS
1	A	209	THR
1	A	215	GLU
1	A	233	GLU
1	A	277	GLU
1	A	278	LEU
1	A	291	LYS
1	A	292	LYS
1	A	304	GLN
1	A	306	SER
1	A	345	LYS
1	A	361	LEU
1	A	376	THR
1	A	381	LYS
1	A	406	ILE
1	A	418	VAL
1	A	420	LEU
1	A	424	LEU
1	A	426	ASN
1	A	428	THR
1	A	436	ASP
1	A	467	GLN
1	A	484	SER
1	A	499	SER
1	A	520	SER
1	A	521	GLU
1	A	526[A]	PHE
1	A	526[B]	PHE
1	A	529	GLU
1	A	532	LYS
1	A	540	MET
1	A	602	GLU
1	A	633	GLU

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Mol	Chain	Res	Type
1	A	643	GLN
1	A	648	THR
1	A	652	ILE
1	A	701	VAL
1	A	735	THR
1	A	738	PRO
1	A	746	ARG
1	A	748	VAL
1	A	752	THR
1	A	754	SER
1	A	776	ARG
1	A	800	MET
1	A	809	MET
1	A	814	SER
1	A	819	SER
1	A	826	LYS
1	A	831	THR
1	A	833	ARG
1	A	835	VAL
1	A	843	ILE
1	A	849	ARG
1	A	868	ILE
1	A	869	LEU
1	A	873	GLU
1	A	886	PRO
1	A	891	MET
1	A	905	ASN
1	A	927	ARG
1	A	941	THR
1	A	949	THR
1	A	962	SER
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	137	ASN
1	A	362	ASN
1	A	584	ASN

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Mol	Chain	Res	Type
1	A	716	ASN
1	A	801	GLN
1	A	816	ASN
1	A	839	HIS
1	A	860	ASN
1	A	905	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 ligands are 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	MES	A	1103	-	12,12,12	2.08	2 (16%)	15,16,16	2.79	4 (26%)
4	EPE	A	1106	-	15,15,15	1.95	1 (6%)	19,20,20	1.72	5 (26%)
5	DTT	A	1107	-	7,7,7	1.15	0	4,8,8	1.61	1 (25%)
2	MES	A	1101	-	12,12,12	1.85	1 (8%)	15,16,16	2.06	6 (40%)
3	GOL	A	1104	-	5,5,5	0.71	0	5,5,5	0.60	0
3	GOL	A	1105	-	5,5,5	0.47	0	5,5,5	1.16	0
2	MES	A	1102	-	12,12,12	2.07	2 (16%)	15,16,16	2.00	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
2	MES	A	1103	-	-	1/6/14/14	0/1/1/1
4	EPE	A	1106	-	-	6/9/19/19	0/1/1/1
5	DTT	A	1107	-	-	2/8/8/8	-
2	MES	A	1101	-	-	0/6/14/14	0/1/1/1
3	GOL	A	1104	-	-	4/4/4/4	-
3	GOL	A	1105	-	-	1/4/4/4	-
2	MES	A	1102	-	-	3/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1106	EPE	C10-S	-6.77	1.68	1.77
2	A	1103	MES	C8-S	-6.14	1.69	1.77
2	A	1102	MES	C8-S	-6.11	1.69	1.77
2	A	1101	MES	C8-S	-5.70	1.69	1.77
2	A	1102	MES	O1S-S	2.21	1.51	1.45
2	A	1103	MES	O2S-S	2.05	1.50	1.45

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1103	MES	O2S-S-C8	7.35	117.83	106.73
2	A	1103	MES	C6-C5-N4	5.80	118.93	110.12
2	A	1102	MES	O2S-S-C8	5.49	115.03	106.73
2	A	1101	MES	C6-C5-N4	-4.09	103.91	110.12
2	A	1101	MES	O3S-S-C8	4.00	113.84	106.00
4	A	1106	EPE	O2S-S-C10	3.76	112.40	106.73
2	A	1103	MES	C2-C3-N4	3.71	115.76	110.12
4	A	1106	EPE	O3S-S-C10	3.56	112.98	106.00
4	A	1106	EPE	O3S-S-O2S	-3.25	103.26	111.40
5	A	1107	DTT	O3-C3-C2	3.11	116.11	109.57
2	A	1102	MES	C6-O1-C2	3.06	119.77	109.88
2	A	1103	MES	O3S-S-O1S	-2.85	104.26	111.40
2	A	1101	MES	O2S-S-C8	-2.80	102.50	106.73
2	A	1101	MES	O1S-S-C8	2.61	110.68	106.73
2	A	1102	MES	C6-C5-N4	-2.42	106.45	110.12
2	A	1102	MES	O2S-S-O1S	-2.30	106.35	113.82
2	A	1101	MES	C7-N4-C3	-2.14	105.53	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1106	EPE	C6-C5-N4	2.14	114.96	110.65
2	A	1102	MES	O3S-S-O2S	-2.10	106.16	111.40
4	A	1106	EPE	C5-N4-C3	2.04	113.24	108.84
2	A	1101	MES	O1-C2-C3	-2.01	107.44	111.77

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
3	A	1104	GOL	O1-C1-C2-C3
4	A	1106	EPE	C9-C10-S-O2S
4	A	1106	EPE	C9-C10-S-O3S
5	A	1107	DTT	C2-C3-C4-S4
5	A	1107	DTT	O3-C3-C4-S4
4	A	1106	EPE	N4-C7-C8-O8
3	A	1104	GOL	C1-C2-C3-O3
4	A	1106	EPE	C10-C9-N1-C2
4	A	1106	EPE	C10-C9-N1-C6
3	A	1104	GOL	O1-C1-C2-O2
3	A	1104	GOL	O2-C2-C3-O3
3	A	1105	GOL	O2-C2-C3-O3
4	A	1106	EPE	C9-C10-S-O1S
2	A	1103	MES	N4-C7-C8-S

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1103	MES	3	0
2	A	1102	MES	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	999/1010 (98%)	0.03	48 (4%) 35 35	37, 66, 132, 167	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	527	PRO	8.0
1	A	989	CYS	5.5
1	A	306	SER	4.4
1	A	900	TYR	4.2
1	A	924	LEU	4.2
1	A	944	LEU	4.0
1	A	437	ASP	4.0
1	A	528[A]	TYR	3.7
1	A	314	ALA	3.5
1	A	531	GLY	3.5
1	A	831	THR	3.4
1	A	174	LYS	3.4
1	A	424	LEU	3.4
1	A	315	ASN	3.3
1	A	908	MET	3.2
1	A	929	TYR	3.2
1	A	1004	TYR	3.0
1	A	987	VAL	3.0
1	A	526[A]	PHE	2.9
1	A	533	VAL	2.9
1	A	435	LYS	2.8
1	A	532	LYS	2.7
1	A	423	THR	2.7
1	A	832	ARG	2.7
1	A	534	PHE	2.7
1	A	988	LEU	2.6
1	A	365	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	173	LYS	2.5
1	A	909	TYR	2.5
1	A	379	LYS	2.3
1	A	529	GLU	2.3
1	A	940	TRP	2.3
1	A	642	LYS	2.2
1	A	956	ARG	2.2
1	A	420	LEU	2.2
1	A	945	VAL	2.2
1	A	380	GLY	2.2
1	A	864	VAL	2.2
1	A	752	THR	2.1
1	A	804	LYS	2.1
1	A	895	MET	2.1
1	A	530	GLY	2.1
1	A	923	GLU	2.1
1	A	809	MET	2.1
1	A	361	LEU	2.1
1	A	854	LEU	2.1
1	A	947	ILE	2.1
1	A	95	LYS	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
4	EPE	A	1106	15/15	0.84	0.24	101,117,134,136	0
3	GOL	A	1104	6/6	0.91	0.17	86,106,110,114	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MES	A	1103	12/12	0.91	0.22	93,132,145,149	0
3	GOL	A	1105	6/6	0.92	0.17	74,76,83,92	0
2	MES	A	1102	12/12	0.93	0.16	73,87,95,97	0
5	DTT	A	1107	8/8	0.94	0.14	99,114,124,132	0
2	MES	A	1101	12/12	0.96	0.11	48,64,72,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.